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Kinetics of the gas-phase reactions of OH radicals with alkanes and cycloalkanes

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Abstract

The available database concerning rate constants for gas-phase reactions of the hydroxyl (OH) radical with alkanes through early 2003 is presented ove the entire temperature range for which measurements have been made (~180–2000 K). Measurements made using relative rate methods are re-evaluated using recent rate data for the reference compound (generally recommendations from this review). In general, whenever more than one study has been carried out over an overlapping temperature range, recommended rate constants or temperature-dependent rate expressions are presented.

1. Introduction

Large quantities of volatile organic compounds (VOCs) are emitted into the atmosphere from anthropogenic and biogenic sources, and a large number of VOCs are present in ambient air (including those formed in situ from the atmospheric reactions of other VOCs). In the troposphere, VOCs can be transformed by photolysis (at wavelengths ?290 nm), reaction with hydroxyl (OH) radicals (mainly during daylight hours), reaction with nitrate (NO_3) radicals (during evening and nighttime hours), and reaction with ozone (O_3) (Atkinson, 2000).

Alkanes are an important class of VOCs (Calvert et al., 2002) which in the atmosphere react with OH radicals and, to a lesser extent, with NO_3 radicals (Atkinson, 2000). Rate constants for the gas-phase reactions of OH radicals with alkanes have been periodically reviewed and evaluated (Atkinson, 1986, 1989, 1994, 1997), and the reactions of OH radicals with $\leq C_4$ alkanes are included in the ongoing NASA (2003) and IUPAC (2003) data evaluations (which are now only available on the World Wide Web, at the locations given in NASA (2003) and IUPAC, 2003). This review and evaluation continues the previous reviews and evaluations of Atkinson (1986, 1989, 1994, 1997), and employs the same general format.

For each alkane and cycloalkane for which experimental kinetic data are available in

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the readily accessible literature, these rate constants are listed. In the table associated with each reaction, the experimental techniques used are denoted by the abbreviations listed in Table 1. For example, use of a flash photolysis system to generate OH radicals with resonance fluorescence monitoring of OH radicals is denoted by PF-RF. When relative rate methods (denoted in the "Technique" column by "RR") were used, the rate constant for the reference compound from the most recent review and evaluation is used to re-evaluate the rate constant for the alkane in question (which therefore may be different from that cited in the original publication). For relative rate studies, the rate constant used for the reference reaction to place the measured rate constant ratio(s) on an absolute basis is noted, and is that recommended from this evaluation (including the rate constants derived in this review and evaluation for the reactions of OH radicals with H_2 and CO), unless noted otherwise.

For absolute rate studies, the temperature-dependent rate expressions are also given (if cited), either as the Arrhenius expression $k = Ae^{-B/T}$ (in which case no entry is given in the column labeled n) or as the three-parameter expression $k = AT^n e^{-B/T}$. When rate constants have been measured over a range of temperatures, Arrhenius plots of ln k vs $1/T$ often exhibit curvature (Atkinson, 1986, 1989, 1994, 1997), and hence the recommended temperature-dependent expressions are then given in terms of the three-parameter expression $k = CT^n e^{-D/T}$ rather than the Arrhenius expression $k = Ae^{-B/T}$. Generally a value of $n = 2$ is used (Atkinson, 1986, 1989, 1994, 1997), resulting in the expression $k = CT^2 e^{-D/T}$. At any given temperature T, an Arrhenius expression can be derived from the three-parameter expression $k = CT^n e^{-D/T}$, with $A = Ce^n T^n$ and $B = D + nT$. While an Arrhenius expression may be adequate over short temperature ranges, extrapolation outside of the temperature range for which the Arrhenius expression is valid is likely to result in significant errors in the predicted rate constant.

The available rate data, from both absolute and relative rate measurements, for the reactions of OH radicals with alkanes and cycloalkanes are reviewed and evaluated

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in the following sections. For the reactions of OH radicals with methane, ethane and propane (and for CH_3D and CD_4), the recommendations are based solely on absolute rate measurements. However, for the $>C_3$ alkanes and for the cycloalkanes, rate constants obtained from relative rate studies are an important part of the data-base (and in some cases are the only data available), and the recommendations then use a combination of absolute and relative rate data. As shown in Table 2, for a series of C_3–C_{10} *n*-alkanes and cyclohexane at room temperature the relative rate studies of Atkinson et al. (1982a, b), Benhke et al. (1987, 1988), Nolting et al. (1988) and DeMore and Bayes (1999) are in generally excellent agreement, and these relative rate studies severely constrain room temperature rate constant recommendations for the $\geq C_5$ *n*-alkanes once rate constants for propane and *n*-butane are recommended from absolute (or mainly absolute) studies.

There are a number of alkanes for which the OH radical reaction rate constants have been measured relative to those for the reactions of OH radicals with H_2 or CO, often at elevated temperatures.

$$OH + H_2 \rightarrow H_2O + H$$

$$OH + CO \rightarrow H + CO_2$$

The available rate constants for these two reactions have been reviewed and evaluated to obtain temperature, and in the case of the CO reaction, pressure dependent rate expressions in order to place the measured rate constant ratios on an absolute basis. For the reaction of OH radicals with H_2, the absolute rate constants measured by Tully and Ravishankara (1980), Ravishankara et al. (1981), Bott and Cohen (1989), Oldenborg et al. (1992) and Talukdar et al. (1996) have been fitted to the three-parameter expression $k = AT^2e^{-B/T}$ to obtain

$$k(H_2)=9.61 \times 10^{-18}T^2e^{-1457/T}\ cm^3\ molecule^{-1}\ s^{-1}$$

over the temperature range 238–1548 K.

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The rate constant for the reaction of OH radicals with CO is temperature and pressure dependent (and with the pressure dependence depending on the specific diluent gas used), with the effect of pressure decreasing as the temperature increases. The kinetics of this reaction have been investigated and evaluated by Golden et al. (1998), with the recommended rate constant being derived from the experimental data using an RRKM model. In this review and evaluation, a simpler (and somewhat more approximate) rate expression analogous to that used previously (Atkinson, 1989) has been derived from the recommended experimental rate constants tabulated by Golden et al. (1998), of

$$k(\mathrm{CO}) = 9.1 \times 10^{-19} T^{1.77} e^{580/T} [1 + 2.4 \times 10^{-20} [\mathrm{M}] (T/298)^{-1}] \, \mathrm{cm^3 \, molecule^{-1} \, s^{-1}}$$

over the temperature range ~290–3000 K and for the pressures encountered in this review article, where [M] is the concentration of M = air, O_2 or N_2 in molecule cm^{-3}. Because of the greater uncertainties in the rate constant for this reaction (as a function of temperature, pressure and diluent gas), rate constants obtained from experimental studies using the reaction of OH radicals with CO as the reference reaction are given relatively low weight in the evaluations, or are not used if other rate data are available.

The estimated uncertainties in the recommended 298 K rate constants are subjective and are in the range ±20–30%. However, it is considered unlikely that future new rate data will change many of the room temperature rate constants by more than 10%; this is approximately the change that has occurred in recommended rate constants for alkanes since the Atkinson (1986) review, with recommended rate constants for most alkanes decreasing by ~10% since 1986.

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2. Rate data for alkanes and cycloalkanes

2.1. OH + methane

The available rate data are listed in Table 3. The recent studies of Bott and Cohen (1989), Vaghjiani and Ravishankara (1991), Finlayson-Pitts et al. (1992), Lancar et al. (1992), Dunlop and Tully (1993), Mellouki et al. (1994), Gierczak et al. (1997) and Bonard et al. (2002) are in good agreement, as shown by the Arrhenius plot in Fig. 1. However, over the temperature range ~250–420 K the rate constants measured in these studies are significantly lower than most of the earlier absolute measurements (Atkinson, 1994). Gierczak et al. (1997) fit their data and the earlier data of Vaghjiani and Ravishankara (1991) from the same laboratory to a three-parameter expression, and obtained the rate expression $k(\text{methane}) = 1.85 \times 10^{-20} T^{2.82} e^{-987/T}$ cm^3 molecule^{-1} s^{-1}. This rate expression is plotted as the solid line in the Arrhenius plot (Fig. 1), and provides an excellent fit to the data of Bott and Cohen (1989), Vaghjiani and Ravishankara (1991), Finlayson-Pitts et al. (1992), Lancar et al. (1992), Dunlop and Tully (1993), Mellouki et al. (1994), Gierczak et al. (1997) and Bonard et al. (2002), agreeing with the 1234 K rate constant of Bott and Cohen (1989) to within 1% and with the 800 K rate constant of Dunlop and Tully (1993) and the 295–668 K rate constants of Bonard et al. (2002) to within 10%. Accordingly, the rate expression of Gierczak et al. (1997) is recommended, with

$k(\text{methane}) = 1.85 \times 10^{-20} T^{2.82} e^{-987/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 190–1240 K, and with

$k(\text{methane}) = 6.40 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.

The overall uncertainty in the rate constant at 298 K is estimated to be ±20%.

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2.2. OH + methane-d_1

The available rate data are listed in Table 4, and Fig. 2 shows an Arrhenius plot of the rate constants of Gordon and Mulac (1975), DeMore (1993a), Gierczak et al. (1997) and Saueressig et al. (2001). The relative rate constants of DeMore (1993a) are slightly higher than those of Gierczak et al. (1997), by up to ~20% at 360 K. The rate constants of DeMore (1993a), Gierczak et al. (1997) and Saueressig et al. (2001) have been fitted to the three parameter expression $k = AT^2e^{-B/T}$, leading to the recommendation of

$k(\text{methane}-d_1)=5.19 \times 10^{-18}T^2e^{-(1332\pm54)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 240–430 K, where the indicated error in B is two least-squares standard deviations, and with

$k(\text{methane}-d_1)=5.28 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.

The overall uncertainty in the rate constant at 298 K is estimated to be ±20%. The recommended rate expression is shown as the solid line in Fig. 2.

2.3. OH + methane-d_2

As shown in Table 5, rate constants are available only from the studies of Gordon and Mulac (1975) and Gierczak et al. (1997), with only one temperature-dependent study (Gierczak et al., 1997). The rate constant of Gordon and Mulac (1975) at 416 K is ~40% higher than predicted from extrapolation of the Arrhenius expression of Gierczak et al. (1997). In the absence of further studies, the Arrhenius expression of Gierczak et al. (1997) should be used (but only over the temperature range 270–360 K).

2.4. OH + methane-d_3

As shown in Table 6, rate constants are available only from the studies of Gordon and Mulac (1975) and Gierczak et al. (1997), with only one temperature-dependent study

(Gierczak et al., 1997). The rate constant of Gordon and Mulac (1975) at 416 K is in reasonable agreement with that predicted from extrapolation of the Arrhenius expression of Gierczak et al. (1997). In the absence of further studies, the Arrhenius expression of Gierczak et al. (1997) should be used (but only in the temperature range 270–360 K).

2.5. OH + methane-d_4

The available rate data are listed in Table 7. Figure 3 shows an Arrhenius plot of the absolute rate constants measured by Gordon and Mulac (1975), Dunlop and Tully (1993) and Gierczak et al. (1997). The rate constant of Gordon and Mulac (1975) at 416 K is a factor of 2 lower than those of Dunlop and Tully (1993) and Gierczak et al. (1997), which are in excellent agreement over the temperature range common to both studies (293–413 K). The rate constants of Dunlop and Tully (1993) and Gierczak et al. (1997) have been fitted to the three parameter expression $k = AT^2e^{-B/T}$, leading to the recommendation of

$$k(\text{methane}-d_4)=5.70 \times 10^{-18} T^2 e^{-(1882\pm32)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

over the temperature range 240–800 K, where the indicated error in B is two least-squares standard deviations, and with

$$k(\text{methane}-d_4)=9.16 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$$

The overall uncertainty in the rate constant at 298 K is estimated to be ±20%. As seen from the Arrhenius plot in Fig. 3, the recommendation underpredicts the rate constants at the two lowest temperatures (244 and 250 K) employed by Gierczak et al. (1997) by 20–25%. Use of a T^3 dependence in the pre-exponential factor makes little difference, with $k(\text{methane}-d_4)=4.91 \times 10^{-21} T^3 e^{-(1478\pm24)/T}$ cm^3 molecule^{-1} s^{-1}, $k(\text{methane-}d_4) = 9.11 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K, and the predicted rate constant at 244 K is 14% lower than the measured value of Gierczak et al. (1997).

2.6. OH + ethane

The available rate data are listed in Table 8. Over the temperature range ~200–800 K the absolute rate constants of Overend et al. (1975), Howard and Evenson (1976b), Leu (1979), Lee and Tang (1982), Margitan and Watson (1982), Tully et al. (1983, 1986a), Smith et al. (1984), Devolder et al. (1984), Schmidt et al. (1985), Baulch et al. (1985), Stachnik et al. (1986), Bourmada et al. (1987), Wallington et al. (1987), Lafage et al. (1987), Zabarnick et al. (1988), Abbatt et al. (1990), Schiffman et al. (1991), Dóbé et al. (1991, 1992), Sharkey and Smith (1993), Talukdar et al. (1994), Crowley et al. (1996), Donahue et al. (1996, 1998) and Clarke et al. (1998) are in good agreement. Because several of these studies involved measurement of the rate constant for the reaction of OH radicals with ethane at one temperature (generally room temperature) as a check on the experimental technique used (Leu, 1979; Lee and Tang, 1982; Margitan and Watson, 1982; Devolder et al., 1984; Bourmada et al., 1987; Lafage et al., 1987; Zabarnick et al., 1988; Dóbé et al., 1991, 1992), the rate constants from the more extensive absolute studies of Tully et al. (1983, 1986a), Smith et al. (1984), Stachnik et al. (1986), Wallington et al. (1987), Abbatt et al. (1990), Talukdar et al. (1994), Donahue et al. (1996, 1998) and Clarke et al. (1998), together with the elevated temperature rate constants of Bott and Cohen (1991a) and Koffend and Cohen (1996), are shown in the Arrhenius plot in Fig. 4. The agreement is seen to be generally excellent, and a least-squares analysis of the rate data of Smith et al. (1984), Tully et al. (1986a) (which is taken to supersede the earlier study of Tully et al., 1983), Stachnik et al. (1986), Wallington et al. (1987), Abbatt et al. (1990), Bott and Cohen (1991a), Talukdar et al. (1994), Koffend and Cohen (1996), Donahue et al. (1996, 1998) and Clarke et al. (1998), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$$k(\text{ethane}) = 1.49 \times 10^{-17} T^2 e^{-(499\pm14)/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$$

over the temperature range 180–1230 K, where the indicated error in B is two least-squares standard deviations, and

$k(\text{ethane}) = 2.48 \times 10^{-13}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K.

The overall uncertainty in the rate constant at 298 K is estimated to be ±20%. The recommended rate expression is shown as the solid line in the Arrhenius plot in Fig. 4. The rate constants measured by Crowley et al. (1996) at 247, 294 and 303 K to check for systematic errors in a newly constructed apparatus are in good agreement with the recommended rate expression, being within 4% of the recommendation at 294 and 303 K and within 12% of the recommendation at 247 K.

The elevated temperature rate constants derived from the relative rate studies of Baldwin et al. (1970b) (as re-evaluated by Baldwin and Walker, 1979) and Hucknall et al. (1975) are in reasonable agreement with the recommendation, to within 7% and 15%, respectively, thereby suggesting that the rate data from these two relative rate studies can be used with some confidence in the evaluations of rate data for other alkanes (see also the discussion of the rate constant for the propane reaction).

2.7. OH + ethane-d_3 and ethane-d_6

The available rate data are listed in Tables 9 (ethane-d_3) and 10 (ethane-d_6). The only study of these reactions to date is that of Tully et al. (1986a). The data of Tully et al. (1986a) for ethane, ethane-d_3 and ethane-d_6 show that the CH_3 and CD_3 groups can be treated independent of whether the neighboring group is a CH_3 or CD_3 group. Thus, to a good approximation the rate constant for CH_3CD_3 is given by 0.5[k(ethane) + k(ethane-d_6)], with a deuterium isotope effect of

$$k_H/k_D[= k(\text{ethane})/k(\text{ethane}-d_6)] = (1.01 \pm 0.06)e^{(456\pm27)/T}$$

over the temperature range 293–705 K, and with $k_H/k_D = 4.61 \pm 0.56$ at 293 K (Tully et al. (1986a).

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2.8. OH + propane

The available rate data are listed in Table 11. The absolute rate constants measured over the temperature range 190–800 K by Tully et al. (1983), Droege and Tully (1986a) (which is viewed as superseding the earlier study of Tully et al., 1983), Nielsen et al. (1988), Abbatt et al. (1990), Mac Leod et al. (1990), Schiffman et al. (1991), Talukdar et al. (1994), Mellouki et al. (1994), Donahue et al. (1998), Clarke et al. (1998), Carl and Crowley (2001) and Kozlov et al. (2003) are in generally good agreement. The data from the more extensive studies of Droege and Tully (1986a), Abbatt et al. (1990), Mac Leod et al. (1990), Talukdar et al. (1994), Mellouki et al. (1994), Donahue et al. (1998), Clarke et al. (1998) and Kozlov et al. (2003) and the higher temperature data of Bott and Cohen (1984) and Smith et al. (1985) are shown in the Arrhenius plot in Fig. 5. A least-squares analysis of the data of Bott and Cohen (1984), Smith et al. (1985), Droege and Tully (1986a), Abbatt et al. (1990), Mac Leod et al. (1990), Talukdar et al. (1994), Mellouki et al. (1994), Donahue et al. (1998) and Clarke et al. (1998), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$$k(\text{propane}) = 1.65 \times 10^{-17} T^2 e^{-(87\pm18)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

over the temperature range 190–1220 K, where the indicated error in the value of B is two least-squares standard deviations, and

$$k(\text{propane}) = 1.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$$

The overall uncertainty in the rate constant at 298 K is estimated to be ±20%. The recommended rate constant expression is shown in the Arrhenius plot as the solid line (Fig. 5). The rate constants measured recently by Kozlov et al. (2003) agree with the recommendation to within 5% over the entire temperature range studied (210–480 K).

The rate constants derived from the relative rate studies of Baker et al. (1970) (as re-evaluated by Baldwin and Walker, 1979), Hucknall et al. (1975), Atkinson et al. (1982b), Edney et al. (1986), Behnke et al. (1987), Finlayson-Pitts et al. (1993) and DeMore

and Bayes (1999) are in generally excellent agreement with the recommendation, to within 7%, 5%, 2%, 3%, 15%, 4% and 8%, respectively. The rate constants derived from the relative rate measurements of DeMore and Bayes (1999) trend from being 2% higher than the recommendation at 428 K to being 7% lower than the recommendation at 227 K. This good agreement of the relative rate data of Baldwin and Walker (1979) (a re-evaluation of the earlier study of Baker et al., 1970), Hucknall et al. (1975), Atkinson et al. (1982b), Edney et al. (1986), Behnke et al. (1987) and DeMore and Bayes (1999) with absolute rate constant data means that these relative rate studies can be used with some confidence in the evaluations of rate data for $\geq C_4$ alkanes for which fewer absolute rate studies have been carried out.

An Arrhenius plot of the absolute and relative rate data of Talukdar et al. (1994), Mellouki et al. (1994), Clarke et al. (1998), DeMore and Bayes (1999) and Kozlov et al. (2003) for temperatures < 300 K is shown in Fig. 6. The agreement is excellent, with the largest disagreement with the recommended expression (shown by the solid line) being 7% and with, for reference, the lowest temperature measurement by Clarke et al. (1998) at 190 K being 4% higher than the recommendation (and well within the stated 7% measurement uncertainty cited by Clarke et al., 1998).

2.9. OH + propane-d_2, propane-d_3, propane-d_5, propane-d_6 and propane-d_8

The available rate data are listed in Tables 12 (propane-d_2), 13 (propane-d_3), 14 (propane-d_5), 15 (propane-d_6) and 16 (propane-d_8). To date, the only study of these reactions is that of Droege and Tully (1986a). The data obtained for propane, propane-d_2, propane-d_3, propane-d_5, propane-d_6 and propane-d_8 show that the CH_3, CH_2, CD_3 and CD_2 groups can be treated as having rate constants which are independent of the isotopic nature of the neighboring group(s) (Droege and Tully, 1986a). Using the k_H/k_D ratio for CH_3/CD_3 groups obtained from the rate data for ethane, ethane-d_3 and ethane-d_6 (Tully et al., 1986a; see reactions above), Droege and Tully (1986a) derived rate constants for H-atom abstraction from the primary C–H bonds of the two CH_3

groups ($2k_{primary}$) and from the secondary C–H bonds in the CH_2 groups ($k_{secondary}$), of

$2k_{primary} = 1.75 \times 10^{-14} T^{0.97} e^{-798/T}$ cm^3 molecule^{-1} s^{-1}

$2k_{primary} = 3.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K

and

$k_{secondary} = 7.76 \times 10^{-17} T^{1.61} e^{18/T}$ cm^3 molecule^{-1}s^{-1}

$k_{secondary} = 7.9 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Droege and Tully (1986a) also derived the deuterium isotope effect for H-/D-atom abstraction from secondary CH_2 or CD_2 groups, of

$k_H/k_D(CH_2/CD_2 \text{ groups}) = (1.13 \pm 0.19) e^{(262 \pm 78)/T}$

over the temperature range 295–854 K, with

$k_H/k_D(CH_2/CD_2 \text{ groups}) = 2.62 \pm 0.49$ at 295 K.

2.10. OH + *n*-butane

The available rate data are listed in Table 17. The absolute rate constant measurements carried out over the temperature range 231–509 K by Schmidt et al. (1985), Droege and Tully (1986b), Abbatt et al. (1990), Schiffman et al. (1991), Talukdar et al. (1994), Donahue et al. (1998) and Chuong and Stevens (2002) are in good agreement, with earlier absolute rate measurements of Greiner (1970), Perry et al. (1976) and Paraskevopoulos and Nip (1980) at room temperature being ~10–15% higher than these more recent studies. Figure 7 shows an Arrhenius plot of the absolute rate constants of Droege and Tully (1986b), Abbatt et al. (1990), Talukdar et al. (1994) and Donahue et al. (1998) together with the relative rate data of Baker et al. (1970) (as re-evaluated by Baldwin and Walker, 1979), Hucknall et al. (1975) and DeMore and Bayes

(1999). A least-squares fit of these data (Hucknall et al., 1975; Baldwin and Walker, 1979; Droege and Tully, 1986b; Abbatt et al., 1990; Talukdar et al., 1994; Donahue et al., 1998; DeMore and Bayes, 1999), using the expression $k = AT^2e^{-B/T}$, results in the recommendation of

$$k(n\text{–butane}) = 1.81 \times 10^{-17} T^2 e^{(114\pm22)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

over the temperature range 230–760 K, where the indicated error in the value of B is two least-squares standard deviations, and

$$k(n\text{–butane}) = 2.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$$

The overall uncertainty in the rate constant is estimated to be ±20% at 298 K. The recommended rate constant expression is shown as the solid line in the Arrhenius plot (Fig. 7).

While the rate constants derived from relative rate studies of Atkinson et al. (1981) and Atkinson and Aschmann (1984) agree with the recommendation within the experimental uncertainties, these rate constants (Atkinson et al., 1981; Atkinson and Aschmann, 1984) for the n-butane reaction were measured relative to that for reaction of the OH radical with propene, with the rate constant ratio of ∼10 being outside of the range (∼0.2–5) of highest accuracy.

2.11. OH + *n*-butane-d_{10}

The available rate data are listed in Table 18. The room temperature rate constant of Paraskevopoulos and Nip (1980) is 20–25% lower than those of Droege and Tully (1986b), which is the only temperature-dependent study to date. Combining their rate constants for *n*-butane and *n*-butane-d_{10} with the deuterium isotope ratio k_H/k_D obtained for the ethane reaction (Tully et al., 1986a), and using the fraction of the overall OH radical reaction proceeding by H-atom abstraction from the secondary CH_2 groups in *n*-butane estimated by Atkinson (1986), Droege and Tully (1986b) derived rate con-

stants for H-atom abstraction from the primary C–H bonds of the two CH_3 groups ($2k_{primary}$) and from the secondary C–H bonds in the two CH_2 groups ($2k_{secondary}$), of

$$2k_{primary} = 6.86 \times 10^{-17} T^{1.73} e^{-379/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$2k_{primary} = 3.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}$$

and

$$2k_{secondary} = 1.20 \times 10^{-16} T^{1.64} e^{124/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$2k_{secondary} = 2.08 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$$

Droege and Tully (1986b) also derived the deuterium isotope effect for H-/D-atom abstraction from secondary CH_2 or CD_2 groups, of

$$k_H/k_D(CH_2/CD_2 \text{ groups}) = (1.31 \pm 0.12) e^{(196 \pm 33)/T}$$

over the temperature range 294–509 K, with

$$k_H/k_D(CH_2/CD_2 \text{ groups}) = 2.52 \pm 0.17 \text{ at } 294 \text{ K}.$$

This deuterium isotope ratio of $k_H/k_D(CH_2/CD_2$ groups) obtained from the *n*-butane and *n*-butane-d_{10} reactions is essentially identical to the ratio of 2.62±0.49 at 295 K obtained from the propane, propane-d_2, propane-d_3, propane-d_5, propane-d_6 and propane-d_8 reactions (Droege and Tully, 1986a).

2.12. OH + 2-methylpropane

The available rate data are listed in Table 19. The absolute rate constants measured over the temperature range 213–864 K by Tully et al. (1986b), Schiffman et al. (1991), Talukdar et al. (1994) and Donahue et al. (1998) are in good agreement. Figure 8 shows an Arrhenius plot of the absolute rate constants of Tully et al. (1986b), Bott

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and Cohen (1989), Talukdar et al. (1994) and Donahue et al. (1998) (no precise temperature was specified in the Schiffman et al., 1991 study) together with the relative rate data of Baker et al. (1970) (as re-evaluted by Baldwin and Walker, 1979), Hucknall et al. (1975) and Atkinson et al. (1984). The agreement is good and a least-squares analysis of these data (Hucknall et al., 1975; Baldwin and Walker, 1979; Atkinson et al., 1984; Tully et al., 1986b; Bott and Cohen, 1989; Talukdar et al., 1994; Donahue et al., 1998), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$$k(\text{2–methylpropane}) = 1.17 \times 10^{-17} T^2 e^{(213\pm24)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

over the temperature range 210–1150 K, where the indicated error in the value of B is two least-squares standard deviations, and

$$k(\text{2–methylpropane}) = 2.12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$$

The overall uncertainty in the rate constant is estimated to be ±20% at 298 K. The recommended rate constant expression is also shown as the solid line in the Arrhenius plot (Fig. 8).

2.13. OH + 2-methylpropane-d_1, 2-methylpropane-d_9 and 2-methylpropane-d_{10}

The available rate data are listed in Tables 20 (2-methylpropane-d_1), 21 (2-methylpropane-d_9) and 22 (2-methylpropane-d_{10}). To date, the only study of these reactions is that of Tully et al. (1986b). Combining their rate constants for 2-methylpropane, 2-methylpropane-d_1, 2-methylpropane-d_9 and 2-methylpropane-d_{10} with the deuterium isotope ratio $k_H/k_D(CH_3/CD_3$ groups) obtained from the 2,2-dimethylpropane (neopentane) reaction (Tully et al., 1985, 1986a), Tully et al. (1986b) derived rate constants for H-atom abstraction from the primary C–H bonds of the three CH_3 groups ($3k_{primary}$) and from the tertiary C–H bond in the CH group ($k_{tertiary}$), of

$$3k_{primary} = 3.81 \times 10^{-16} T^{1.53} e^{-391/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$3k_{primary} = 6.3 \times 10^{-13} cm^3$ molecule^{-1} s^{-1} at 298 K

and

$k_{tertiary} = 9.52 \times 10^{-14} T^{0.51} e^{-32/T}$ cm^3 molecule^{-1} s^{-1}

$k_{tertiary} = 1.56 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Tully et al. (1986b) also derived the deuterium isotope effect for H-/D-atom abstraction from the tertiary CH or CD group, of k_H/k_D(CH/CD group) = 1.91 at 294 K.

2.14. OH + *n*-pentane

The available rate data are listed in Table 23. The absolute rate studies of Abbatt et al. (1990), Talukdar et al. (1994) and Donahue et al. (1998) are in good agreement at room temperature, and those of Talukdar et al. (1994) and Donahue et al. (1998) agree well over the temperature range common to both studies (300-370 K). However, rate constants derived from the relative rate studies of Atkinson et al. (1982b), Behnke et al. (1987, 1988), Harris and Kerr (1988), Donaghy et al. (1993) and DeMore and Bayes (1999) are consistently ~10% lower that the absolute rate constants. Figure 9 shows an Arrhenius plot of the absolute rate constants of Abbatt et al. (1990), Talukdar et al. (1994) and Donahue et al. (1998) together with the relative rate data of Baldwin and Walker (1979), Atkinson et al. (1982b), Harris and Kerr (1988) and DeMore and Bayes (1999). An appreciable amount of scatter in the data is apparent, both between and within the various studies. A least-squares analysis of the rate constants from these studies (Baldwin and Walker, 1979; Atkinson et al., 1982b; Harris and Kerr, 1988; Abbatt et al., 1990; Talukdar et al., 1994; Donahue et al., 1998; DeMore and Bayes, 1999), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(*n*–pentane)=$2.52 \times 10^{-17} T^2 e^{(158\pm40)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 220–760 K, where the indicated error in the value of B is two least-squares standard deviations, and

$k(n\text{–pentane}) = 3.80 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K.

The overall uncertainty in the rate constant at 298 K is estimated to be ±25%. The recommended rate constant expression is shown as the solid line in the Arrhenius plot (Fig. 9). In the temperature range 224–390 K, the absolute rate constants are generally slightly higher than the recommendation, while the relative rate constants of Harris and Kerr (1988) and DeMore and Bayes (1999) are slightly lower than the recommendation. Obviously, additional data are needed over the entire temperature range of ~200–1000 K.

2.15. OH + 2-methylbutane

The available rate data are listed in Table 24. Rate constants have only been measured at room temperature using relative rate studies (Lloyd et al., 1976; Darnall et al., 1978; Cox et al., 1980; Atkinson et al., 1984), and exhibit a significant amount of scatter. The most recent and extensive study of Atkinson et al. (1984) is used to recommend that

$k(2\text{–methylbutane}) = 3.6 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$

at 298 K, with an estimated overall uncertainty of ±30%.

2.16. OH + 2,2-dimethylpropane

The available rate data are listed in Table 25, and the data-base is relatively small. Figure 10 shows an Arrhenius plot of the data of Greiner (1970), Baker et al. (1976) (as re-evaluated by Baldwin and Walker, 1979), Paraskevopoulos and Nip (1980), Atkinson et al. (1982a), Tully et al. (1986a) and Nielsen et al. (1991b). Clearly, at room temperature the measured rate constants show an appreciable amount of scatter, ranging from 7.0×10^{-13} cm^3 molecule^{-1} s^{-1} to 9.1×10^{-13} cm^3 molecule^{-1} s^{-1}. In particular,

there is a discrepancy between the 299 K rate constant derived from the relative rate study of Atkinson et al. (1982a) (the data of which are in excellent agreement with absolute and relative rate studies for other alkanes) and the absolute rate constant at 287 K measured by Tully et al. (1986a).

A least-squares analysis of the relative rate constants of Baker et al. (1976) (as reevaluated by Baldwin and Walker, 1979) and Atkinson et al. (1982a) and the absolute rate constants of Tully et al. (1986a), using the expression $k = AT^2e^{-B/T}$, results in the recommendation of

$$k(2,2\text{–dimethylpropane}) = 1.86 \times 10^{-17} T^2 e^{-(207\pm56)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

over the temperature range 280–910 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

$$k(2,2\text{–dimethylpropane}) = 8.25 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K},$$

with an estimated uncertainty at 298 K of ±20%. This recommended expression is shown in the Arrhenius plot by the solid line (Fig. 10).

2.17. OH + 2,2-dimethylpropane-d_{12}

As shown in Table 26, the only study of this reaction to date is that of Tully et al. (1985, 1986a). From their rate constants for 2,2-dimethylpropane and 2,2,-dimethylpropane-d_{12}, Tully et al. (1986a) obtained the deuterium isotope ratio for H- (or D-) atom abstraction from CH_3 and CD_3 groups of

$$k_H/k_D(\text{CH}_3/\text{CD}_3 \text{ groups}) = (0.94 \pm 0.09)e^{(472\pm47)/T}$$

over the temperature range 287–903 K. At 298 K, $k_H/k_D(\text{CH}_3/\text{CD}_3$ groups) = 4.6, identical to the value (4.61 ± 0.56 at 293 K) derived from the ethane, ethane-d_3 and ethane-d_6 reactions (Tully et al., 1986a).

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2.18. OH + *n*-hexane

The available rate data are listed in Table 27, and to date only two absolute rate studies have been carried out, that of Koffend and Cohen (1996) at 962 K and that of Donahue et al. (1998) over the temperature range 300–390 K. Furthermore, the only temperature-dependent studies are the absolute rate study of Donahue et al. (1998) (300–390 K) and the relative rate study of DeMore and Bayes (1999) (292–397 K), with no rate constants having been measured below 290 K.

Figure 11 shows an Arrhenius plot of the absolute rate constants of Koffend and Cohen (1996) and Donahue et al. (1998) together with the relative rate data of Atkinson et al. (1982a), Klein et al. (1984) and DeMore and Bayes (1999). In the temperature range 292–390 K the agreement between the absolute and relative rate studies is good. The room temperature relative rate data of Atkinson et al. (1983a), Atkinson and Aschmann (1984), Behnke et al. (1987, 1988) and McLoughlin et al. (1993), which are not shown in the Arrhenius plot in Fig. 11, are also in good agreement with these data of Atkinson et al. (1982a), Klein et al. (1984), Donahue et al. (1998) and DeMore and Bayes (1999). However, as shown by the dashed line in the Arrhenius plot (Fig. 11), a least-squares analysis of the rate constants from the studies of Atkinson et al. (1982a), Klein et al. (1984), Koffend and Cohen (1996), Donahue et al. (1998) and DeMore and Bayes (1999) using the expression $k = AT^2e^{-B/T}$ leads to a rate constant expression of k(*n*-hexane)= $1.82 \times 10^{-17} T^2 e^{361/T}$ cm^3 molecule^{-1} s^{-1} over the temperature range 290–970 K, which does not fit the data particularly well.

A least-squares analysis of the rate constants in the temperature range 292–390 K of Atkinson et al. (1982a), Klein et al. (1984), Donahue et al. (1998) and DeMore and Bayes (1999) using the Arrhenius expression $k = Ae^{-B/T}$ leads to

$$k(n\text{–hexane}) = 2.29 \times 10^{-11} e^{-(442 \pm 52)/T} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1},$$

where the indicated error in the value of B is two least-squares standard deviations,

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and

$k(n\text{–hexane}) = 5.20 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K.

A least-squares analysis of the rate constants of Atkinson et al. (1982a), Klein et al. (1984), Koffend and Cohen (1996), Donahue et al. (1998) and DeMore and Bayes (1999) using the expression $k = ATe^{-B/T}$ leads to

$k(n\text{–hexane}) = 2.54 \times 10^{-14} T e^{-(112 \pm 28)/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$

over the temperature range 290–970 K, where the indicated error in the value of B is two least-squares standard deviations, and

$k(n\text{–hexane}) = 5.20 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

with an estimated overall uncertainty at 298 K of ±20%. This expression is shown as the solid line in Fig. 11. The Arrhenius expression $k(n\text{-hexane}) = 2.29 \times 10^{-11} e^{-442/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ and the expression $k(n\text{-hexane}) = 2.54 \times 10^{-14} T e^{-112/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ lead to rate constants which agree to within 1% over the temperature range 280–390 K; the use of either expression outside of this temperature range 280–390 K may be unreliable.

Provisionally, the rate expression

$k(n\text{–hexane}) = 2.54 \times 10^{-14} T e^{-112/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$

is recommended for the temperature range 290–970 K, although additional data at temperatures >400 K are needed. In particular, it is necessary to confirm the 962 K rate constant of Koffend and Cohen (1996), which appears low by comparison with the recommendation for *n*-pentane.

2.19. OH + 2-methylpentane

As shown in Table 28, rate constants for 2-methylpentane are available only at room temperature from relative rate studies. The rate constants derived from the studies of

Lloyd et al. (1976), Cox et al. (1980) and Atkinson et al. (1984) are in agreement within their stated uncertainties. The most recent and extensive study of Atkinson et al. (1984) is used to recommend that

k(2–methylpentane)=5.2 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}

at 298 K, with an estimated uncertainty of ±25%.

2.20. OH + 3-methylpentane

As shown in Table 29, rate constants for 3-methylpentane are available only at room temperature from relative rate studies. The rate constants derived from the studies of Lloyd et al. (1976) and Atkinson et al. (1984) are in agreement within their stated uncertainties. The most recent and extensive study of Atkinson et al. (1984) is used to recommend that

k(3–methylpentane)=5.2 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1}

at 298 K, with an estimated uncertainty of ±25%.

2.21. OH + 2,2-dimethylbutane

As shown in Table 30, rate constants are available only from the relative rate studies of Atkinson et al. (1984) and Harris and Kerr (1988). At room temperature the rate constants from these two studies (Atkinson et al., 1984; Harris and Kerr, 1988) are in agreement within their stated uncertainties. Figure 12 shows an Arrhenius plot of the rate constants of Atkinson et al. (1984) and Harris and Kerr (1988). Within the scatter of the data, the plot is a good straight line, and a least-squares analysis of the data of Atkinson et al. (1984) and Harris and Kerr (1988) leads to the Arrhenius expression of

k(2, 2–dimethylbutane)=3.37 × $10^{-11}e^{-(809\pm84)/T}$ cm^3 $molecule^{-1}$ s^{-1}

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over the temperature range 240–330 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

$k(2,2\text{–dimethylbutane}) = 2.23 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

with an estimated uncertainty at 298 K of ±25%. This recommended Arrhenius expression, which should not be used outside of the temperature range 240–330 K, is shown as the solid line in the Arrhenius plot (Fig. 12). As noted previously (Atkinson, 1989), the temperature dependence of this rate constant (B = 809 K) is higher than the estimated value (B = 445 K for the temperature range 245–328 K, Kwok and Atkinson, 1995), and needs to be confirmed.

2.22. OH + 2,3-dimethylbutane

As shown in Table 31, few kinetic studies are available for this reaction, and the available rate constants show significant scatter. Figure 13 shows an Arrhenius plot of the absolute rate constants of Greiner (1970) and Bott and Cohen (1991b) together with the rate constants derived from the relative rate studies of Atkinson et al. (1982a) and Harris and Kerr (1988). The absolute room temperature rate constant of Greiner (1970) is ~25–30% higher than the relative rate data of Atkinson et al. (1982a) and Harris and Kerr (1988), and the temperature dependence obtained by Greiner (1970) is negative. The rate constants derived from the relative rate study of Harris and Kerr (1988) exhibit a fair amount of scatter and many also have significant stated uncertainties (two standard deviations of up to ±20%). Accordingly, the absolute 1220 K rate constant of Bott and Cohen (1991b) and the 299 K relative rate constant of Atkinson et al. (1982a) have been used with the expression $k = AT^2e^{-B/T}$ to obtain the recommendation of

$k(2,3\text{–dimethylbutane}) = 1.66 \times 10^{-17} T^2 e^{407/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$

with

$k(2,3\text{–dimethylbutane}) = 5.78 \times 10^{-12}\ \text{cm}^3\ \text{molecule}^{-1}\text{s}^{-1}$ at 298 K,

and with an estimated overall uncertainty at 298 K of ±25%. This expression is shown in the Arrhenius plot as the solid line (Fig. 13), and fits the Harris and Kerr (1988) data reasonably well (although the Harris and Kerr (1988) rate data are consistent with a zero temperature dependence over the range 247–327 K), being ∼10% higher than the Harris and Kerr (1988) rate constants at 325–327 K.

2.23. OH + *n*-heptane

As shown in Table 32, the database for this reaction is small, with the only absolute rate study being that Koffend and Cohen (1996) at 1086 K (note that, assuming that the experimental data listed in their Table III is correct, then the temperature is incorrectly stated in both the abstract and Table VII of Koffend and Cohen (1996) as 1186 K). The room temperature rate constants are all from relative rate studies (Atkinson et al., 1982b; Klöpffer et al., 1986; Behnke et al., 1987, 1988; Ferrari et al., 1996). A least-squares analysis of the rate constants from the studies of Atkinson et al. (1982b), Behnke et al. (1987, 1988), Koffend and Cohen (1996) and Ferrari et al. (1996), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(*n*–heptane)=$1.95 \times 10^{-17} T^2 e^{406/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–1090 K, and

k(*n*–heptane)=6.76×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated overall uncertainty at 298 K of ±20%.

2.24. OH + 2,4-dimethylpentane

As shown in Table 33, the only study of this reaction to date is that of Atkinson et al. (1984).

2.25. OH + 2,2,3-trimethylbutane

The available rate data are listed in Table 34. The only absolute rate study of this reaction is that of Greiner (1970), with the rate constants being quite scattered and that at room temperature being ~25% higher than the relative rate data of Darnall et al. (1976), Atkinson et al. (1984) and Harris and Kerr (1988). The rate constants derived from the relative rate study of Harris and Kerr (1988) with 2,2-dimethylbutane as the reference compound are subject to large uncertainties (~20–30%) and are also highly variable (as are those using *n*-pentane as the reference compound, though to a lesser extent).

Figure 14 shows an Arrhenius plot of the rate constants of Greiner (1970), Baldwin et al. (1981), Atkinson et al. (1984) and Harris and Kerr (1988). Using the relative rate constants of Baldwin et al. (1981) and Atkinson et al. (1984) and the rate expression $k = AT^2e^{-B/T}$ leads to the recommendation of

k(2, 2, 3–trimethylbutane)=$9.20 \times 10^{-18} T^2 e^{459/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–760 K, and

k(2, 2, 3–trimethylbutane)=3.81×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated overall uncertainty at 298 K of ±25%. This recommended rate constant is shown as the solid line in the Arrhenius plot (Fig. 14). While the rate constants of Harris and Kerr (1988) obtained relative to those for *n*-pentane and 2,2-dimethylbutane are highly scattered, the rate constants of Harris and Kerr (1988) relative to those for *n*-hexane are in excellent agreement (to within 5% and within their stated uncertainties) with the recommended expression over the temperature range 243–324 K (Fig. 14).

2.26. OH + *n*-octane

The available rate data are listed in Table 35, with only two absolute rate studies (Greiner, 1970; Koffend and Cohen, 1996) and three room temperature relative rate

measurements (Atkinson et al., 1982b; Behnke et al., 1987; Nolting et al., 1988) having been carried out. Figure 15 shows an Arrhenius plot of the absolute rate constants of Greiner (1970) and Koffend and Cohen (1996) together with the relative rate data of Atkinson et al. (1982b), Behnke et al. (1987) and Nolting et al. (1988). The three relative rate measurements (Atkinson et al., 1982b; Behnke et al., 1987; Nolting et al., 1988) are in excellent agreement, and a least-squares analysis of the rate constants from the studies of Atkinson et al. (1982b), Behnke et al. (1987) and Koffend and Cohen (1996) (the study of Nolting et al., 1988 was not used in the evaluation because the *n*-octane rate constant is used to derive the *n*-heptane rate constant which was the reference compound in the Nolting et al., 1988 study), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$k(n\text{–octane}) = 2.72 \times 10^{-17} T^2 e^{361/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–1080 K, and

$k(n\text{–octane}) = 8.11 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated overall uncertainty at 29 K of ±20%. This rate expression is shown as the solid line in the Arrhenius plot (Fig. 15). The rate constant obtained relative to *n*-heptane by Nolting et al. (1988) at 312 K is in excellent agreement with the recommendation.

2.27. OH + 2,2,4-trimethylpentane

As shown in Table 36, few studies of the kinetics of this reaction have been carried out. Figure 16 shows an Arrhenius plot of the rate constants of Greiner (1970), Atkinson et al. (1984) and Bott and Cohen (1991b). At room temperature the agreement between the studies of Greiner (1970) and Atkinson et al. (1984) is good. Using the relative rate constant of Atkinson et al. (1984) and the 1186 K absolute rate constant of Bott and Cohen (1991b) and the rate expression $k = AT^2e^{-B/T}$ leads to the recommendation of

$k(2,2,4\text{–trimethylpentane}) = 2.35 \times 10^{-17} T^2 e^{140/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–1190 K, and

$k(2,2,4\text{–trimethylpentane}) = 3.34 \times 10^{-12}\ \text{cm}^3\text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

with an estimated overall uncertainty at 298 K of ±20%. This recommended rate constant is shown as the solid line in the Arrhenius plot (Fig. 16). The absolute rate constants of Greiner (1970) are in generally good agreement with this recommendation, and a least-squares analysis of the rate constants of Greiner (1970), Atkinson et al. (1984) and Bott and Cohen (1991b) leads to the rate constant k(2,2,4-trimethylpentane)= $2.10 \times 10^{-17} T^2 e^{190/T}$ cm^3 molecule^{-1} s^{-1} over the same temperature range of 290–1190 K, with k(2,2,4-trimethylpentane)= 3.53×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K.

2.28. OH + 2,3,4-trimethylpentane

As shown in Table 37, the only study of this reaction to date is that of Harris and Kerr (1988).

2.29. OH + 2,2,3,3-tetramethylbutane

As shown in Table 38, few studies of the kinetics of this reaction have been carried out. Figure 17 shows an Arrhenius plot of the rate constants of Greiner (1970), Baldwin et al. (1979), Atkinson et al. (1984), Tully et al. (1985) and Bott and Cohen (1991b). The agreement at room temperature between the studies of Greiner (1970), Atkinson et al. (1984) and Tully et al. (1985) is good. A least-squares analysis of the relative rate constants of Baldwin et al. (1979) (these data also being given in Baldwin and Walker, 1979) and Atkinson et al. (1984) and the absolute rate constants of Tully et al. (1985) and Bott and Cohen (1991b), using the rate expression $k = AT^2 e^{-B/T}$, leads to the recommendation of

$k(2,2,3,3\text{–tetramethylbutane}) = 1.99 \times 10^{-17} T^2 e^{-(178\pm123)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–1180 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

$k(2,2,3,3\text{–tetramethylbutane}) = 9.72 \times 10^{-13}\,\text{cm}^3\,\text{molecule}^{-1}\,\text{s}^{-1}$ at 298 K,

with an estimated overall uncertainty at 298 K of ±20%. This recommended rate constant is shown as the solid line in the Arrhenius plot (Fig. 17). The absolute rate constants of Greiner (1970) are in generally good agreement with this recommendation.

2.30. OH + *n*-nonane

The available rate data are listed in Table 39. The room temperature rate constants for *n*-nonane are all from relative rate studies (Atkinson et al., 1982b; Behnke et al., 1987, 1988; Nolting et al., 1988; Ferrari et al., 1996; Kramp and Paulson, 1998), and are in good agreement. A least-squares analysis of the rate constants of Atkinson et al. (1982b), Behnke et al. (1987, 1988), Nolting et al. (1988), Koffend and Cohen (1996), Ferrari et al. (1996) and Kramp and Paulson (1998), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$k(n\text{–nonane}) = 2.53 \times 10^{-17} T^2 e^{(436\pm34)/T}\,\text{cm}^3\,\text{molecule}^{-1}\,\text{s}^{-1}$

over the temperature range 290–1100 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

$k(n\text{–nonane}) = 9.70 \times 10^{-12}\,\text{cm}^3\,\text{molecule}^{-1}\,\text{s}^{-1}$ at 298 K,

with an estimated overall uncertainty at 298 K of ±20%. The relative rate constant of Coeur et al. (1998, 1999) is in agreement, within the apparently sizeable error limits, with the recommendation.

2.31. OH + 3,3-diethylpentane

As shown in Table 40, the only study of this reaction to date is that of Nielsen et al. (1991b). The absolute and relative rate measurements of Nielsen et al. (1991b) agree

within their stated experimental uncertainties. A rate constant of

k(3, 3–diethylpentane)=4.8 × 10^{-12} cm^3 $molecule^{-1}$ s^{-1} at 298 K

is recommended, with an estimated overall uncertainty of ±25%.

2.32. OH + *n*-decane

As shown in Table 41, the available room temperature rate constants for n-decane are all from relative rate studies (Atkinson et al., 1982b; Nolting et al., 1988; Behnke et al., 1988; Aschmann et al., 2001), and are in good agreement. A least-squares analysis of the rate constants of Atkinson et al. (1982b), Nolting et al. (1988), Behnke et al. (1988), Koffend and Cohen (1996) and Aschmann et al. (2001), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(*n*–decane)=3.17 × $10^{-17}T^2e^{(406\pm56)/T}$ cm^3 $molecule^{-1}$ s^{-1}

over the temperature range 290–1110 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

k(*n*–decane)=1.10 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 298 K,

with an estimated overall uncertainty at 298 K of ±20%.

2.33. OH + 3,4-diethylhexane

As shown in Table 42, the only study of this reaction to date is that of Aschmann et al. (2001).

2.34. OH + *n*-undecane

As evident from Table 43, the room temperature rate constants derived from the relative rate studies of Nolting et al. (1988) and Behnke et al. (1988) are in good agreement.

An average of these two rate constants (Nolting et al., 1988; Behnke et al., 1988) leads to the recommendation of

$k(n\text{–undecane}) = 1.23 \times 10^{-11}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

by extrapolating the 312 K and 300 K rate constants to 298 K using a reasonable value of B (425 K) and with an estimated overall uncertainty at 298 K of ±20%.

2.35. OH + *n*-dodecane

As evident from Table 44, the room temperature rate constants derived from the relative rate studies of Nolting et al. (1988) and Behnke et al. (1988) are in good agreement. An average of these two rate constants leads to the recommendation of

$k(n\text{–dodecane}) = 1.32 \times 10^{-11}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

by extrapolating the 312 K and 300 K rate constants to 298 K using a reasonable value of B (425 K) and with an estimated overall uncertainty at 298 K of ±20%.

2.36. OH + *n*-tridecane

As shown in Table 45, the room temperature rate constants derived from the relative rate studies of Nolting et al. (1988) and Behnke et al. (1988) are in good agreement. An average of these two rate constants leads to the recommendation of

$k(n\text{–tridecane}) = 1.51 \times 10^{-11}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

by extrapolating the 312 K and 300 K rate constants to 298 K using a reasonable value of B (425 K) and with an estimated overall uncertainty at 298 K of ±25%.

2.37. OH + *n*-tetradecane, *n*-pentadecane and *n*-hexadecane

As shown in Tables 46 (*n*-tetradecane), 47 (*n*-pentadecane) and 48 (*n*-hexadecane), the only study of these reactions to date is that of Nolting et al. (1988).

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2.38. OH + cyclopropane

The available rate data are listed in Table 49. Rate constants are available from the absolute rate studies of Jolly et al. (1985), Dóbé et al. (1991, 1992) and Clarke et al. (1998) and from the relative rate studies of DeMore and Bayes (1999) and Wilson et al. (2001). Figure 18 shows an Arrhenius plot of the data from these studies (for the study of Wilson et al. (2001) only the data obtained relative to the rate constant for ethane are plotted). The absolute rate constants of Dóbé et al. (1991, 1992) are significantly higher than the other data, more so at room temperature, with the discrepancy decreasing as the temperature increases (Fig. 18). Accordingly, the data of Dóbé et al. (1991, 1992) are not used in the evaluation of the rate constant for this reaction. While this discrepancy could be due to the presence of reactive impurities in the cyclopropane sample used by Dóbé et al. (1991, 1992), Dóbé et al. (1991, 1992) stated that the cyclopropane sample was ≥99.99% pure with 0.01% propene impurity (Dóbé et al., 1992) (which would result in a ∼4% increase in the measured rate constant at 298 K). The room temperature rate constants of Jolly et al. (1985), Clarke et al. (1998), DeMore and Bayes (1999) and Wilson et al. (2001) are in good agreement. However, as evident from the Arrhenius plot (Fig. 18), the absolute rate constants of Clarke et al. (1998) over the temperature range 200–360 K exhibit a lower temperature dependence than do the relative rate data of DeMore and Bayes (1999) and Wilson et al. (2001) over the temperature range 276–463 K.

A least-squares analysis of the rate constant data of Jolly et al. (1985), Clarke et al. (1998), DeMore and Bayes (1999) and Wilson et al. (2001) (relative to ethane; while the rate constants obtained by Wilson et al. (2001) relative to ethane agree with those obtained relative to CH_3CHF_2 (to within ∼ ±10%), due to the larger uncertainty in the rate constant for the reaction of OH radicals with CH_3CHF_2 only the rate constants relative to ethane are used in the evaluation), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

$$k(\text{cyclopropane}) = 4.21 \times 10^{-18} T^2 e^{-(454\pm87)/T}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$$

over the temperature range 200–460 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

$k(\text{cyclopropane}) = 8.15 \times 10^{-14}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$ at 298 K,

with an estimated uncertainty at 298 K of +10%, −30%. This recommended expression is shown in the Arrhenius plot as the solid line (Fig. 18). Obviously, further data are needed at temperatures <290 K to better assess the temperature dependence of the rate constant in the range 200–300 K. The significantly different temperature dependencies obtained by Clarke et al. (1998) and by DeMore and Bayes (1999) and Wilson et al. (2001) lead to the recommended rate expression giving an ∼10% higher calculated 298 K rate constant than measured by Jolly et al. (1985), Clarke et al. (1998), DeMore and Bayes (1999) and Wilson et al. (2001).

2.39. OH + isopropylcyclopropane

As evident from Table 50, the only study of this reaction to date is that of Atkinson and Aschmann (1988).

2.40. OH + cyclobutane

As shown in Table 51, rate constants are available from the absolute rate studies of Dóbé et al. (1991, 1992) and from the relative rate studies of Gorse and Volman (1974) and DeMore and Bayes (1999). Figure 19 shows an Arrhenius plot of the data from these studies. The room temperature rate constant of Gorse and Volman (1974) obtained relative to that for the reaction of OH radicals with CO is significantly lower than the rate constants of Dóbé et al. (1991, 1992) and DeMore and Bayes (1999), and is not used in the evaluation of the rate constant for this reaction. While the temperature dependencies obtained by Dóbé et al. (1991, 1992) and DeMore and Bayes (1999) are similar, the rate constants of DeMore and Bayes (1999) are uniformly ∼15% higher than those of Dóbé et al. (1991, 1992) (Fig. 19). Because of the good agreement of the relative rate data of DeMore and Bayes (1999) with absolute and relative rate constants for

other alkanes and cycloalkanes, the data of DeMore and Bayes (1999) are preferred, despite their rate constants being the highest. Accordingly, a least-squares analysis of the rate constants of DeMore and Bayes (1999), using the expression $k = AT^2e^{-B/T}$, results in the recommendation of

k(cyclobutane)=$2.10 \times 10^{-17} T^2 e^{(25\pm81)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 270–370 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

k(cyclobutane)=2.03×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated uncertainty at 298 K of ±30%. This recommended expression is shown in the Arrhenius plot as the solid line (Fig. 19). Obviously, further data are needed.

2.41. OH + cyclopentane

The available rate data are listed in Table 52. Rate constants are available from the absolute rate studies of Jolly et al. (1985), Droege and Tully (1987), Bott and Cohen (1989) and Donahue et al. (1998) and from the relative rate studies of Volman (1975), Darnall et al. (1978), Atkinson et al. (1982a), Kramp and Paulson (1998) and DeMore and Bayes (1999). The study of Atkinson et al. (1982a) is judged to supersede the earlier study of Darnall et al. (1978), and Fig. 20 shows an Arrhenius plot of the data of Atkinson et al. (1982a), Jolly et al. (1985), Droege and Tully (1987), Bott and Cohen (1989), Kramp and Paulson (1998), Donahue et al. (1998) and DeMore and Bayes (1999). There is an appreciable amount of scatter in the measured room temperature rate constants, with the rate constant of Kramp and Paulson (1998) relative to 1,3-butadiene being lower than the other rate data, and the absolute rate constants of Donahue et al. (1998) are both quite scattered and generally higher than the rate constants of Atkinson et al. (1982a), Jolly et al. (1985), Droege and Tully (1987),

Kramp and Paulson (1998) (including those relative to *n*-nonane, propene and *trans*-2-butene), and DeMore and Bayes (1999). A least-squares analysis of the rate constants of Atkinson et al. (1982a), Jolly et al. (1985), Droege and Tully (1987), Bott and Cohen (1989), Kramp and Paulson (1998), Donahue et al. (1998) and DeMore and Bayes (1999), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(cyclopentane)=2.73 × $10^{-17}T^2e^{(214\pm45)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 270–1200 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

k(cyclopentane)=4.97 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated uncertainty at 298 K of ±25%. This recommended expression is shown in the Arrhenius plot as the solid line (Fig. 20).

A least-squares analysis of the rate constants of Atkinson et al. (1982a), Jolly et al. (1985), Droege and Tully (1987), Bott and Cohen (1989), Kramp and Paulson (1998) (only the rate constants relative to *n*-nonane, propene and *trans*-2-butene, because of the possibility that 1,3-butadiene reacted significantly with NO_2 and/or O(^{3}P) atoms, Kramp and Paulson, 1998) and DeMore and Bayes (1999), using the expression $k = AT^2e^{-B/T}$, leads to k(cyclopentane)=2.64 × $10^{-17}T^2e^{(219\pm21)/T}$ cm^3 molecule^{-1} s^{-1} over the temperature range 270–1200 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and k(cyclopentane)=4.89 × 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (i.e. within 3% of the recommended expression over the temperature range 270–1200 K).

2.42. OH + cyclopentane-d$_{10}$

As shown in Table 53, rate constants for cyclopentane-d$_{10}$ are available only from the absolute rate study of Droege and Tully (1987). Combining their absolute rate constants for cyclopentane-h$_{10}$ (k_H) and cyclopentane-d$_{10}$ (k_D) results in a rate constant

ratio of

$k_H/k_D(CH_2/CD_2$ groups$)=(1.16 \pm 0.10)e^{(254\pm16)/T}$

over the temperature range 295–491 K, with

$k_H/k_D(CH_2/CD_2$ groups$)=2.74 \pm 0.17$ at 295 K.

This temperature-dependent expression for k_H/k_D and the ratio at room temperature are similar to the deuterium isotope ratios $k_H/k_D(CH_2/CD_2$ groups) obtained by Droege and Tully (1986a) for the propane reactions ($k_H/k_D(CH_2/CD_2$ groups) $= (1.13 \pm 0.19)e^{(262\pm78)/T}$ over the temperature range 295–854 K, $k_H/k_D(CH_2/CD_2$ groups) $= 2.62 \pm 0.49$ at 295 K), by Droege and Tully (1986b) for the *n*-butane reactions ($k_H/k_D(CH_2/CD_2$ groups) $= (1.31 \pm 0.12)e^{(196\pm33)/T}$ over the temperature range 294–509 K, $k_H/k_D(CH_2/CD_2$ groups) $= 2.52 \pm 0.17$ at 294 K) and by Droege and Tully (1987) for the cyclohexane reactions ($k_H/k_D(CH_2/CD_2$ groups) $= (1.16 \pm 0.06)e^{(237\pm10)/T}$ over the temperature range 292–491 K, $k_H/k_D(CH_2/CD_2$ groups) $= 2.59 \pm 0.16$ at 292 K).

2.43. OH + cyclohexane

The available rate data are listed in Table 54. Rate constants are available from the absolute rate studies of Greiner (1970), Nielsen et al. (1986), Bourmada et al. (1987), Droege and Tully (1987), Saunders et al. (1994) and Donahue et al. (1996, 1998), and from a number of relative rate studies (Gorse and Volman, 1974; Wu et al., 1976; Atkinson et al., 1982a, 1983b; Tuazon et al., 1983; Edney et al., 1986; Japar et al., 1990; Atkinson and Aschmann, 1992; Sommerlade et al., 1993; DeMore and Bayes, 1999). Most of these rate constants have been measured only at room temperature. There is an appreciable amount of scatter in the room temperature rate constants, which range from 5.2×10^{-12} to 8.6×10^{-12} cm^3 molecule^{-1} s^{-1}. Figure 21 shows an Arrhenius plot of the absolute rate constants of Droege and Tully (1987) and Donahue et al. (1998) together with the relative rate constants of Atkinson et al. (1982a, 1983b), Tuazon et

al. (1983), Atkinson and Aschmann (1992) and DeMore and Bayes (1999) (relative to *n*-butane and *n*-pentane; their data relative to propane (DeMore and Bayes, 1999) have not been used because of the relatively high rate constant ratios determined using this reference compound and hence potentially higher uncertainties). The absolute rate constants of Donahue et al. (1998) are seen to be quite scattered (as is also the case for the cyclopentane reaction), and are hence not used in the evaluation. A least-squares analysis of the rate constants of Droege and Tully (1987), Atkinson et al. (1982a, 1983b), Tuazon et al. (1983), Atkinson and Aschmann (1992) and DeMore and Bayes (1999), using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(cyclohexane)=$3.26 \times 10^{-17} T^2 e^{(262\pm33)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–500 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

k(cyclohexane)=6.97×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated uncertainty at 298 K of ±20%. This recommended expression is shown in the Arrhenius plot as the solid line (Fig. 21).

The relative rate data of Japar et al. (1990), Sommerlade et al. (1993), Kramp and Paulson (1998) and those of DeMore and Bayes (1999) relative to propane (not used in the evaluation; see above) are in excellent agreement with the recommended rate constant, while that of Edney et al. (1986) is 20% lower.

2.44. OH + cyclohexane-d_{12}

As evident from Table 55, rate constants for cyclohexane-d_{12} are available only from the absolute rate study of Droege and Tully (1987). Combining their absolute rate constants for cyclohexane-h_{12} (k_H) and cyclohexane-d_{12} (k_D) results in a rate constant ratio of

$k_H/k_D = (1.16 \pm 0.06)e^{(237\pm10)/T}$

over the temperature range 292–491 K, with

$k_H/k_D = 2.59 \pm 0.16$ *at* 292 K.

As noted for the cyclopentane-d_{10} reaction, this temperature-dependent expression for k_H/k_D and the ratio at room temperature are similar to the deuterium isotope ratios $k_H/k_D(CH_2/CD_2$ groups) obtained by Droege and Tully (1986a) for the propane reactions ($k_H/k_D(CH_2/CD_2$ groups) = $(1.13 \pm 0.19)e^{(262\pm78)/T}$ over the temperature range 295–854 K, $k_H/k_D(CH_2/CD_2$ groups) = 2.62 ± 0.49 at 295 K), by Droege and Tully (1986b) for the *n*-butane reactions ($k_H/k_D(CH_2/CD_2$ groups) = $(1.31 \pm 0.12)e^{(196\pm33)/T}$ over the temperature range 294–509 K, $k_H/k_D(CH_2/CD_2$ groups) = 2.52 ± 0.17 at 294 K) and by Droege and Tully (1987) for the cyclopentane reactions ($k_H/k_D(CH_2/CD_2$ groups) = $(1.16 \pm 0.10)e^{(254\pm16)/T}$ over the temperature range 295–491 K, $k_H/k_D(CH_2/CD_2$ groups) = 2.74 ± 0.17 at 295 K).

2.45. OH + methylcyclohexane

As shown in Table 56, the only study of this reaction to date is that of Atkinson et al. (1984).

2.46. OH + *n*-butylcyclohexane

As shown in Table 57, the only study of this reaction to date is that of Aschmann et al. (2001).

2.47. OH + cycloheptane

As shown in Table 58, rate constants for cycloheptane are available only from the absolute rate studies of Jolly et al. (1985) and Donahue et al. (1998). As shown in the Arrhenius plot (Fig. 22), the room temperature rate constants from these two

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studies (Jolly et al., 1985; Donahue et al., 1998) are in good agreement. A least-squares analysis of the rate constants from these two studies, using the expression $k = AT^2e^{-B/T}$, leads to the recommendation of

k(cycloheptane)=$3.99 \times 10^{-17} T^2 e^{(373\pm119)/T}$ cm^3 molecule^{-1} s^{-1}

over the temperature range 290–390 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and

k(cycloheptane)=1.24×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K,

with an estimated uncertainty at 298 K of ±25%. This recommended expression is shown in the Arrhenius plot as the solid line (Fig. 22).

2.48. OH + cyclooctane

As evident from Table 59, the only study of this reaction to date is that of Donahue et al. (1998). A least-squares analysis of the rate constants of Donahue et al. (1998), using the expression $k = AT^2e^{-B/T}$, leads to k(cyclooctane)=$5.91 \times 10^{-17} T^2 e^{(276\pm143)/T}$ cm^3 molecule^{-1} s^{-1} over the temperature range 300–390 K, where the indicated uncertainty in the value of B is two least-squares standard deviations, and with k(cyclooctane)=1.33×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K.

2.49. OH + bicyclo[2.2.1]heptane, bicyclo[2.2.2]octane and bicyclo[3.3.0]octane

As shown in Tables 60 (bicyclo[2.2.1]heptane), 61 (bicyclo[2.2.2]octane) and 62 (bicyclo[3.3.0]octane), the only study of these reactions to date is that of Atkinson et al. (1983c).

2.50. OH + *cis*-bicyclo[4.3.0]nonane and *trans*-bicyclo[4.3.0]nonane

As shown in Tables 63 (*cis*-bicyclo[4.3.0]nonane) and 64 (*trans*-bicyclo[4.3.0]nonane), the only study of these reactions to date is that of Atkinson

et al. (1983c). The rate constant ratio k(*cis*-bicyclo[4.3.0]nonane)/k(*trans*-bicyclo[4.3.0]nonane) was determined to be 0.966±0.014 at 299±2 K (Atkinson et al., 1983c).

2.51. OH + *cis*-bicyclo[4.4.0]decane and *trans*-bicyclo[4.4.0]decane

As shown in Tables 65 (*cis*-bicyclo[4.4.0]decane) and 66 (*trans*-bicyclo[4.3.0]decane), the only study of these reactions to date is that of Atkinson et al. (1983c). The rate constant ratio k(*cis*-bicyclo[4.4.0]decane)/k(*trans*-bicyclo[4.4.0]decane) was determined to be 0.976±0.021 at 299±2 K (Atkinson et al., 1983c).

2.52. OH + tricyclo[5.2.1.$0^{2,6}$]decane and tricyclo[3.3.1.$1^{3,7}$]decane

As shown in Tables 67 (tricyclo[5.2.1.$0^{2,6}$]decane) and 68 (tricyclo[3.3.1.$1^{3,7}$]decane), the only published study of these reactions to date is that of Atkinson et al. (1983c).

2.53. OH + *trans*-pinane, tricyclene and quadricyclane

As shown in Tables 69 (*trans*-pinane), 70 (tricyclene) and 71 (quadricyclane), the only study of these reactions to date is that of Atkinson and Aschmann (1992).

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Table 1. List of abbreviations used in tables of rate data, under "Technique" column

Abbreviation	Experimental Technique
FP	Flash photolysis
DF	Discharge flow
PLP	Pulsed laser photolysis
RR	Relative rate
PR	Pulse radiolysis
LH	Laser heating
SH	Shock heating (shock tube)
RA	Resonance absorption
RF	Resonance fluorescence
KS	Kinetic spectroscopy
MMS	Molecular modulation-spectroscopy
LIF	Laser induced fluorescence
MS	Mass spectrometry
EPR	Electron paramagnetic resonance
LMR	Laser magnetic resonance

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Table 2. Relative rate constants for a series of alkanes at room temperature

alkane	Atkinson et al. (1982a, b) (299±2 K)	Behnke et al. (1987) (300±3 K)	Nolting et al. (1988) (312 K)	Behnke et al. (1988) (300 K)	DeMore and Bayes (1999) (298 K)
propane	0.473±0.016	0.539			0.467
n-butane	1.00	1.00		1.00	1.00
n-pentane	1.60±0.04	1.62	(1.60)[a]	1.63±0.04	1.57
n-hexane	2.21±0.04	2.19	2.31±0.24	2.24±0.04	2.19
n-heptane	2.83±0.07	2.78	2.80±0.11	2.88±0.06	
n-octane	3.49±0.07	3.37	3.28±0.17	3.46±0.06	
n-nonane	4.13±0.13	4.07	3.80±0.19	4.06±0.11	
n-decane	4.42±0.22		4.36±0.23	4.88±0.11	
cyclohexane	2.91±0.10				2.86
	2.93±0.02				

[a] Based on the data cited in the table from the studies of Atkinson et al. (1982b), Behnke et al. (1987, 1988) and DeMore and Bayes (1999).

Table 3. Rate constants and temperature-dependent parameters for the reaction of OH radicals with methane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			21±10.5	1650–1840	RR [relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Westenberg and Fristrom (1961)	1650–1840
			12.5	1445	RR[relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Fenimore and Jones (1961)	1220–1800
			12.8	1560			
			11.1	1580			
			12.9	1690			
			16.8	1800			
			0.181	673	RR[relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Hoare (1962)	673–923
			0.256	723			
			0.54	798			
			0.77	873			
			1.03	923			
			26	~1370–1680	RR[relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Fristrom (1963)	~1370–1680
			0.45±0.23	773	RR [relative to k(CO)=2.49 × 10^{-13}]	Blundell et al. (1965)	773–823
			0.185	673	RR[relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Hoare (1966)	673–923
			0.291	723			
			0.54	798			
			0.80	873			
			1.09	923			
			0.59	798	RR[relative to k(CO=2.58 × 10^{-13}]	Hoare and Peacock (1966)	
			0.87±0.18	773	RR [relative to $k(H_2)$ = 8.72 × 10^{-13}]	Baldwin et al. (1967)	
			5.0±1.7	1285	Flame-RA/MS	Dixon-Lewis and Williams (1967)	
			0.0108±0.0025	300	DF-EPR	Wilson and Westenberg (1967)	
			0.00880±0.00034	301±1	FP-KS	Greiner (1967a)	
83		2516	0.0179[a]	298	FP-KS	Horne and Norrish (1967)	298–423
			18±4	1750–2000	RR [relative to k(CO) $= 9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Wilson et al. (1969)	1750–2000

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.96±0.09	773	RR [relative to $k(H_2)$ = 8.72×10^{-13}]	Baldwin et al. (1970a)	
			0.00849±0.00072	295	FP-KS	Greiner (1970)	295–498
			0.00953±0.00029	295			
			0.0106±0.0003	296			
			0.0103±0.0006	296			
			0.00804±0.00020	301			
			0.00805±0.00042	301			
			0.00903±0.00088	302			
			0.0154±0.0006	333			
			0.0352±0.0007	370			
			0.0611±0.0024	424			
			0.121±0.004	492			
			0.120±0.004	493			
			0.121±0.003	493			
			0.113±0.003	497			
5.5		1898±52	0.122±0.003	498			
			$0.185^{+0.185}_{-0.093}$	548	[relative to $k(CO)=1.85 \times 10^{-13}$]	Simonaitis et al. (1971)	
50		3020	6.7[a]	1500	Flame-MS	Peeters and Mahnen (1973)	1100–1900
			0.00185±0.00010	240	FP-RF	Davis et al. (1974)	240–373
			0.00185±0.00017	240			
			0.00495±0.00025	276			
			0.00749±0.00010	298			
			0.0075±0.00075	298			
			0.0069±0.0008	298			
2.36		1711±88	0.0236	373			
			0.00715±0.00042	293	DF-RF	Margitan et al. (1974)	293–427
			0.0212±0.0004	359			
			0.0306±0.0001	384			
			0.0422±0.0018	407			
3.83		1842±21	0.0521±0.0016	427			
			0.0261±0.0027	381	PR-RA	Gordon and Mulac (1975)	381–416
			0.0548±0.0017	416			
			0.00651±0.00027	295±2	FP-RA	Overend et al. (1975)	
			0.0095±0.0014	296±2	DF-LMR	Howard and Evenson (1976a)	

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0088±0.0007	298	FP-RA	Zellner and Steinert (1976)	298–892
			0.0148	330			
			0.020	358			
			0.028	381			
			0.061	444			
			0.070	453			
			0.113	498			
			0.174	525			
			0.257	564			
			0.251±0.033	576			
			0.276±0.033	584			
			0.335	622			
			0.551	629			
			0.822	671			
			0.830	680			
			1.12	738			
			1.21	756			
			1.51	776			
5.76×10^{-9}	3.08	1010	2.71	892			
			0.00638±0.00074	296±2	RR [relative to $k(H_2)$ $= 6.13 \times 10^{-15}$]	Cox et al. (1976)	
			9.0	1300	RR [relative to $k(H_2)$ $= 5.30 \times 10^{-12}$]	Bradley et al. (1976)	
			3.82	1140	SH/FP-RA	Ernst et al. (1978)	1140–1505
			3.82	1160			
			4.48	1165			
			3.49	1188			
			3.49	1192			
			4.82	1203			
			4.15	1220			
			3.82	1245			
			3.99	1260			
			4.15	1260			
			3.49	1265			
			4.48	1270			
			4.65	1270			
			3.82	1275			
			3.99	1275			
			3.99	1303			
			4.32	1313			
			5.65	1335			
			5.31	1404			
			5.15	1410			
			4.48	1415			
			5.65	1500			
			5.31	1505			

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0070±0.0007	296	FP-RA (of CH_3) with computer modeling	Sworski et al. (1980)	
			0.00750±0.00060	298	FR-RF	Tully and Ravishankara (1980)	298–1020
			0.0473±0.0045	398			
			0.081±0.011	448			
			0.145±0.012	511			
			0.167±0.006	529			
			0.314±0.040	600			
			0.275±0.044	619			
			0.578±0.058	696			
			0.84±0.15	772			
			1.50±0.15	915			
1.32×10^{-5}	1.92	1355	2.00±0.20	1020			
			0.00766±0.00064	300	FP-RF	Husain et al. (1981)	
			1.25±0.45	830±50	LH-LIF	Fairchild et al. (1982)	830–1400
			1.3±0.4	1030±50			
			4.3±1.0	1400±50			
			0.00557±0.00054	269	DF-RF	Jeong and Kaufman (1982); Jeong et al. (1984)	269–473
			0.00789±0.00049	297			
			0.0178±0.0012	339			
			0.0347±0.0023	389			
			0.0549±0.0035	419			
1.28×10^{-12}	4.23	453±776	0.102±0.007	473			
			0.0379±0.0032	413	RR [relative to $k(CO)=9.1 \times 10^{-19} T^{1.77} e^{580/T}$]	Baulch et al. (1983)	413–693
			0.0541±0.0064	417			
			0.0350±0.0032	422			
			0.0636±0.0066	443			
			0.0773±0.0068	471			
			0.0963±0.0070	505			
			0.103±0.018	517			
			0.0926±0.0178	521			
			0.112±0.006	546			
			0.166±0.004	553			
			0.275±0.016	603			
			0.366±0.022	663			
			0.627±0.065	693			

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.00650	298	PR-RA	Jonah	298–1229
			0.00846	298		et al. (1984)	
			0.0189	348			
			0.0351	373			
			0.106	398			
			0.0938	415			
			0.175	424			
			0.124	450			
			0.209	483			
			0.174	483			
			0.336	543			
			0.584	571			
			0.545	613			
			0.760	667			
			0.893	709			
			0.991	712			
			1.04	769			
			1.52	858			
			2.48	873			
			2.27	974			
			2.01	974			
			4.50	1071			
			3.22	1125			
			4.19	1125			
			4.93	1229			
			0.0085±0.0006	298±3	FP-RF	Madronich and	298–1512
			0.0228±0.0043	362±10		Felder (1985)	
			0.0463±0.0034	407±5			
			0.0629±0.009	410±14			
			0.154±0.014	510±10			
			0.177±0.017	525±10			
			0.202±0.010	546±5			
			0.439±0.038	626±16			
			0.478±0.07	698±22			
			1.48±0.08	900±12			
			212±0.23	967±35			
			2.16±0.11	1005±15			
			2.72±0.15	1103±17			
			3.34±0.20	1164±17			
			2.41±0.22	1174±22			
			3.18±0.17	1176±17			
			3.89±0.25	1196±17			
			4.26±0.39	1196±37			
			3.77±0.32	1238±18			
			3.68±0.23	1244±17			
			3.58±0.27	1261±23			
			3.80±0.37	1261±18			

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			4.74±0.20	1300±18			
			4.20±0.21	1307±18			
			4.84±0.50	1314±23			
			5.32±0.31	1345±18			
			5.61±0.34	1365±19			
			6.44±0.53	1396±19			
			5.98±0.69	1455±20			
			6.52±1.15	1510±20			
2.57×10^{-5}	1.83	1396±134	6.74±0.35	1512±20			
			3	1220	SH-RA	Bott and Cohen (1985)	
			1.25±0.6	830	LH-LIF	Smith et al. (1985)	830–1412
			2.25±1.0	870			
			1.55±0.7	930			
			2.0±1.0	966			
			2.1±1.2	975			
			1.33±0.5	1030			
			3.6±0.9	1120			
			1.7±0.7	1150			
			2.35±0.7	1176			
			3.3±1.0	1200			
			2.9±0.35	1240			
			4.4±0.8	1400			
			4.2±0.8	1412			
			4.3±0.9	1234±15	SH-RA	Bott and Cohen (1989)	
			0.00093±0.00003	223	PLP-LIF	Vaghjiani and Ravishankara (1991)	223–420
			0.00102±0.00002	223			
			0.00104±0.00002	223			
			0.00097±0.00003	223			
			0.00086±0.00002	223			
			0.00089±0.00003	223			
			0.00086±0.00004	223			
			0.00089±0.00004	223			
			0.00088±0.00004	223			
			0.00103±0.00002	223			
			0.00086±0.00002	223			
			0.00125±0.00002	233			
			0.00133±0.00002	233			
			0.00125±0.00003	233			
			0.00118±0.00002	233			
			0.00118±0.00003	233			
			0.00119±0.00001	233			
			0.00121±0.00002	233			
			0.00182±0.00002	250			
			0.00204±0.00005	250			

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.00198±0.00003	250			
			0.00350±0.00005	273			
			0.00352±0.00007	273			
			0.00338±0.00007	273			
			0.00371±0.00016	273			
			0.00375±0.00005	273			
			0.00367±0.00004	273			
			0.00364±0.00005	273			
			0.00592±0.00018	295			
			0.00647±0.00006	297			
			0.00636±0.00022	297			
			0.00630±0.00007	298			
			0.00620±0.00018	298			
			0.00684±0.00025	303			
			0.00713±0.00018	303			
			0.00674±0.00013	303			
			0.00674±0.00008	303			
			0.00715±0.00011	303			
			0.00712±0.00038	303			
			0.01026±0.00015	325			
			0.01598±0.00011	350			
			0.02617±0.00042	380			
			0.04287±0.00052	420			
			0.04253±0.00052	420			
			0.04244±0.00057	420			
			0.04336±0.00063	420			
			0.04366±0.00056	420			
			0.04184±0.00061	420			
1.59×10^{-8}	2.84	978	0.04304±0.00047	420			
2.94		1815±30					
			0.00409±0.00026	278	DF-RF	Finlayson-Pitts	278–378
			0.00560±0.00063	298		et al. (1992)	
			0.00575±0.00098	298			
			0.0106±0.0017	313			
			0.00792±0.00007	313			
			0.0105±0.0028	333			
			0.0109±0.0006	333			
			0.0150±0.0025	348			
			0.0143±0.0036	348			
			0.0205±0.0019	363			
4.0		1944±114	0.0236±0.0008	378			
			0.0262±0.0027	378	DF-EPR	Lancar	378–422
			0.0427±0.0018	422		et al. (1992)	

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			<0.0003	178±2	PLP-LIF	Sharkey and Smith (1993)	178–298
			0.00165±0.0002	216±2			
			0.0076±0.0003	298±2			
			0.00562±0.00043	293	PLP-LIF	Dunlop and Tully (1993)	293–800
			0.0371±0.0022	409			
			0.0422±0.0023	420			
			0.101±0.004	498			
			0.152±0.010	547			
			0.237±0.014	602			
			0.367±0.022	654			
			0.474±0.026	704			
			0.576±0.032	745			
9.45×10^{-8} [b]	2.58[b]	1082[b]	0.756±0.042	800			
			0.0054±0.0002	292	PLP-LIF	Saunders et al. (1993)	
			0.00132±0.00005	233	PLP-LIF	Mellouki et al. (1994)	233–343
			0.00208±0.00030	243			
			0.00215±0.00030	252			
			0.00370±0.00020	273			
			0.00642±0.00060	295			
			0.00634±0.00056	298			
			0.0105±0.0006	323			
2.56		1765±146	0.0168±0.0015	343			
			0.00036±0.00002	195	FP-LIF	Gierczak et al. (1997)	195–296
			0.00040±0.00002	200			
			0.00049±0.00003	206			
			0.00063±0.00006	213			
			0.00075±0.00007	218			
			0.00082±0.00042	223			
			0.00602±0.00010	295			
			0.00585±0.00022	295			
			0.00590±0.00016	295			
			0.00615±0.00026	295			
1.85×10^{-8} [c]	2.82[c]	987[c]	0.00620±0.00016	296			

Table 3. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.00623±0.00020	295	PLP-LIF	Bonard et al. (2002)	295–668
			0.00916±0.00028	319			
			0.0219±0.0007	367			
			0.0426±0.0018	419			
			0.0783±0.0021	464			
			0.133±0.004	519			
			0.205±0.009	569			
			0.306±0.010	619			
5.65×10^{-9}	3.01	959±36	0.422±0.014	668			

[a] Calculated from the cited Arrhenius expression.
[b] Fit of combined data sets of Dunlop and Tully (1993) and Vaghjiani and Ravishankara (1991) over the temperature range 223–800 K.
[c] Fit of combined data sets of Gierczak et al. (1997) and Vaghjiani and Ravishankara (1991) over the temperature range 195–420 K.

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Table 4. Rate constants and temperature-dependent parameters for the reaction of OH radicals with methane-d_1

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0365±0.0017	416	PR-RA	Gordon and Mulac (1975)	
			0.00588	298	RR [relative to k(methane)	DeMore	298–358
			0.00562	298	$= 1.85 \times 10^{-20} T^{2.82} e^{-987/T}$	(1993a)	
			0.00546	298	from combination of		
			0.00553	298	$k(CH_3D)/k(CH_3CFCl_2)$ and		
			0.00721	308	$k(CH_3CFCl_2/k$(methane)[a])		
			0.00884	318			
			0.0129	338			
			0.0147	348			
			0.0184	358			
			0.0187	358			
			0.00504	293	RR[relative to k(methane)	DeMore	293–361
			0.00550	299	$= 1.85 \times 10^{-20} T^{2.82} e^{-987/T}$	(1993a)	
			0.00608	303	from combination of		
			0.00720	311	$k(CH_3D)/k(CF_3CH_2F)$ and		
			0.00852	320	$k(CF_3CH_2F/k$(methane)[b])		
			0.0104	331			
			0.0127	343			
			0.0143	348			
			0.0145	350			
			0.0181	361			
			0.00150±0.00005	249	FP-LIF	Gierczak et al. (1997)	249–422
			0.00160±0.00016	253			
			0.00183±0.00014	258			
			0.00216±0.00018	263			
			0.00259±0.00013	268			
			0.00284±0.00014	273			
			0.00328±0.00020	278			
			0.00382±0.00020	286			
			0.00448±0.00012	291			
			0.00506±0.00029	298			
			0.00506±0.00029	298			
			0.00505±0.00018	298			
			0.00615±0.00010	307			
			0.00734±0.00014	317			
			0.00935±0.00048	330			
			0.01143±0.00081	343			
			0.01357±0.00060	353			
			0.01564±0.00058	362			
			0.02021±0.00076	376			
			0.02389±0.00057	391			

Table 4. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0281±0.0016	403			
			0.0321±0.0027	413			
1.07×10^{-5}	1.87	1332±20	0.0374±0.0012	422			
			0.00474±0.00007	296	RR [relative to k(methane) = 6.14×10^{-15}]	Saueressig et al. (2001)	

[a] From Huder and DeMore (1993).
[b] From DeMore (1993b).

Table 5. Rate constants and temperature-dependent parameters for the reaction of OH radicals with methane-d_2

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0299±0.0017	416	PR-RA	Gordon and Mulac (1975)	
			0.00160±0.00030	270	PLP-LIF	Gierczak et al. (1997)	270–354
			0.00364±0.00044	297			
			0.00353±0.00034	297			
			0.00559±0.00032	324			
2.18		1926±250	0.00908±0.00054	354			

Table 6. Rate constants and temperature-dependent parameters for the reaction of OH radicals with methane-d_3

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0111±0.0005	416	PR-RA	Gordon and and Mulac (1975)	
			0.00102±0.00004	270	FP/PLP-LIF	Gierczak et al. (1997)	270–354
			0.00171±0.00020	293			
			0.00177±0.00010	295			
			0.00197±0.00004	297			
			0.00328±0.00034	323			
1.46		1972±80	0.00564±0.00020	354			

Table 7. Rate constants and temperature-dependent parameters for the reaction of OH radicals with methane-d_4

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0050±0.0002	416	PR-RA	Gordon and and Mulac (1975)	
			0.00083±0.00008	293	PLP-LIF	Dunlop and Tully (1993)	293–800
			0.00215±0.00018	333			
			0.00422±0.00032	365			
			0.00910±0.00058	409			
			0.0191±0.0011	459			
			0.0306±0.0022	498			
			0.0530±0.0032	547			
			0.0900±0.0056	602			
			0.150±0.010	654			
			0.197±0.012	704			
			0.302±0.018	753			
8.70×10^{-10}	3.23	1334	0.385±0.024	800			
			0.00019±0.00002	244	FP-LIF	Gierczak et al. (1997)	244–413
			0.00023±0.00003	250			
			0.00027±0.00002	259			
			0.00033±0.00002	265			
			0.00039±0.00002	269			
			0.00044±0.00002	276			
			0.00056±0.00006	282			
			0.00066±0.00004	289			
			0.00085±0.00002	296			
			0.00084±0.00004	296			
			0.00086±0.00005	299			
			0.00087±0.00002	300			
			0.00132±0.00005	310			
			0.00156±0.00018	320			
			0.00223±0.00005	333			
			0.00295±0.00008	346			
			0.00367±0.00012	357			
			0.00577±0.00022	380			
			0.00697±0.00018	391			
			0.0101±0.0001	413			
			0.00985±0.00040	413			
5.65×10^{-9}	3.01	1545±15	0.00979±0.00040	413			

Table 8. Rate constants and temperature-dependent parameters for the reaction of OH radicals with ethane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			13.2	813	RR[relative to $k(H_2)$ $= 1.06 \times 10^{-12}$]	Baldwin and Simmons (1957)	
			15.2	1420	RR[relative to	Fenimore and	1420–1610
			17.3	1440	$k(CO) = 9.1 \times 10^{-19}$	Jones (1963)	
			21.0	1600	$T^{1.77} e^{580/T}$]		
			21.0	1600			
			24.9	1610			
			1.7	1300	RR[relative to	Westenberg and	1300–1550
			12	1550	$k(CO) = 9.1 \times 10^{-19}$ $T^{1.77} e^{580/T}$]	and Fristrom (1965)	
209		1812±302	0.478[a]	298	FP-KS	Horne and Norrish (1967)	298–423
			0.292±0.039	302±2	FP-KS	Griner (1967b)	
			≤ 1.0	300	DF-EPR	Wilson and Westenberg (1967)	
			6.0	734	RR[relative to	Hoare and	734–798
			7.2	773	k(methane) = 1.85×	Patel (1969)	
			9.8	798	$10^{-20} T^{2.82} e^{-987/T}$]		
			4.97	773	RR[relative to $k(H_2)$ $= 8.72 \times 10^{-13}$]	Baldwin et al. (1970b); Baldwin and Walker (1979)	
			0.311±0.007	297	FP-KS	Greiner (1970)	297–493
			0.340±0.010	298			
			0.239±0.014	299			
			0.282±0.007	299			
			0.304±0.035	300			
			0.224±0.042	301			
			0.457±0.010	335			
			0.751±0.050	369			
			0.937±0.059	424			
18.6		1232±54	1.55±0.04	493			
			0.664±0.034	381	PR-RA	Gordon and	381–416
			0.797±0.050	416		Mulac (1975)	

Table 8. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.40±0.39	653	RR[rleative to k(methane) = 3.54× 10^{-13}]	Hucknall et al. (1975)	
			0.264±0.017	295±2	FP-RA	Overend et al. (1975)	
			0.290±0.060	296	DF-LMR	Howard and Evenson (1976b)	
			25.9	1300	RR[relative to $k(H_2)$ = 5.30 × 10^{-12}]	Bradley et al. (1976)	
			0.26±0.04	298	DF-RF	Leu (1979)	
			0.231±0.040	295±1	DF-RF	Lee and Tang (1982)	
			0.080	238	FP-RF	Margitan and Watson (1982)	
			0.659±0.048	403	RR[relative to k(CO) = 9.1 × 10^{-19} $T^{1.77} e^{580/T}$]	Baulch et al. (1983)	403–683
			1.17±0.12	443			
			1.27±0.09	493			
			2.52±0.19	561			
			2.29±0.26	595			
			4.73±0.56	683			
			0.259±0.021	297	FP-RF	Tully et al. (1983)	297–800
			0.771±0.076	400			
			1.58±0.10	499			
			2.61±0.33	609			
			3.65±0.25	697			
1.43×10^{-2}	1.05	911	5.07±0.34	800			
			0.196±0.013	248	DF-RF	Jeong et al. (1984)	248–472
			0.228±0.014	273			
			0.310±0.020	294			
			0.306±0.021	298			
			0.426±0.027	333			
			0.403±0.027	333			
			0.538±0.035	375			
			0.529±0.034	375			
			0.799±0.054	428			
			0.770±0.048	429			
			0.993±0.068	464			
3.87×10^{-9} 6.11	3.09	−171 ± 343 886±36	1.03±0.067	472			

Table 8. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
16.1		1173	0.324	300	PR-RA	Nielsen et al. (1984)	300–400
			0.105±0.004	240	FP-RF	Smith et al. (1984)	240–295
			0.147±0.006	251			
			0.205±0.009	273			
18.0		1240±110	0.263±0.010	295			
			0.275	295	DF-RF	Devolder et al. (1984)	
			0.22±0.03	295	PLP-LIF	Schmidt et al. (1985)	
			0.267±0.040	295±2	DF-RF	Baulch et al. (1985)	
			0.239±0.010	292.5	PLP-LIF	Tully et al. (1986a)	292–705
			0.407±0.017	340			
			0.651±0.027	396			
			1.15±0.048	478			
			1.23± 0.051	484			
			2.01±0.083	577			
			2.11±0.088	586			
8.51×10^{-6}	2.06	430	3.48±0.144	705			
			0.298±0.021	295	PR-RA	Nielsen et al. (1986)	
			0.127±0.008	248	PLP-RA	Stachnik et al. (1986)	248–297
			0.129±0.009	248			
			0.251±0.006	297			
			0.250±0.006	297			
			0.31±0.06	295.9±1.2	RR[relative to k(propane)=1.08× 10^{-12}	Edney et al. (1986)	
			0.277±0.03	296±2	DF-RF	Bourmada et al. (1987)	
			0.088±0.013	226	FP-RF	Wallington et al. (1987)	226–363
			0.107±0.010	241			
			0.162±0.018	261			
			0.230±0.026	296			
8.4		1050±100	0.497±0.055	363			
			0.287	294	DF-RF	Lafage et al. (1987)	294–413
			1.12	413			
			0.253	294	DF-LIF	Lafage et al. (1987)	
			0.261±0.013	296	PLP-LIF	Zabarnick et al. (1988)	
			0.238±0.016	297±2	DF-LIF	Abbatt et al. (1990)	

Table 8. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.243±0.012	~ 298[b]	PLP-IR	Schiffman et al. (1991)	
			0.274±0.040	298	PLP-RF	Dóbé et al. (1991, 1992)	
			15.4±2.4	1225±16	SH-RA	Bott and Cohen (1991a)	
			0.013±0.002	138	PLP-LIF	Sharkey and Smith (1993)	138–298
			0.025±0.003	178			
			0.0785±0.004	216			
			0.295±0.014	298			
			0.276±0.007	298	RR[relative to k(propane) = 1.65× $10^{-17}T^2e^{-87/T}$]	Finlayson-Pitts et al. (1993)	298–373
			0.270±0.012	298			
			0.362±0.014	323			
			0.468±0.013	348			
			0.579±0.010	373			
			0.0882±0.0024	231	PLP-LIF	Talukdar et al. (1994)	231–377
			0.1269±0.0069	252			
			0.1303±0.0015	253			
			0.1778±0.0043	273			
			0.2461±0.0032	299			
			0.3380±0.0037	327			
			0.4589±0.0050	355			
1.53×10^{-5}	2	512±7	0.5641±0.0082	377			
10.3		1108±40					
			8.37	974±16	SH-RA	Koffend and Cohen (1996)	
			0.108±0.002	247	PLP-RF	Crowley et al. (1996)	247–303
			0.228±0.004	294			
			0.267±0.003	303			
			0.255±0.03	300	DF-LIF	Donahue et al. (1996)	
			0.259±0.008	300	DF-LIF	Donahue et al. (1998)	298–407
			0.355±0.011	325			
			0.390±0.012	340			
			0.438±0.023	360			
			0.561±0.017	375			
			0.604±0.018	390			

Table 8. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0269±0.0027	180	DF-LIF	Clarke et al. (1998)	180–360
			0.0377±0.0004	190			
			0.0454±0.0025	200			
			0.0651±0.0007	213			
			0.0808±0.0012	225			
			0.0967±0.0018	238			
			0.1251±0.0014	250			
			0.1640±0.0018	265			
			0.2081±0.0016	280			
			0.2515±0.0021	295			
			0.2953±0.0050	310			
			0.3464±0.0037	325			
			0.3744±0.0038	340			
			0.4637±0.0164	360			

[a] Calculated from the cited Arrhenius expression.
[b] Room temperature; assumed to be ~298 K.

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Table 9. Rate constants and temperature-dependent parameters for the reaction of OH radicals with ethane-d_3

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.142±0.007	293	PLP-LIF	Tully et al. (1986a)	293–705
			0.250±0.011	338			
			0.419±0.018	396			
			0.794±0.033	478			
			1.52±0.063	586			
7.65×10^{-7}	2.38	817	2.65±0.110	705			

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Table 10. Rate constants and temperature-dependent parameters for the reaction of OH radicals with ethane-d_6

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0523±0.0060	293	PLP-LIF	Tully et al. (1986a)	293–705
			0.105±0.007	339.5			
			0.199±0.010	396			
			0.435±0.020	478			
			0.965±0.041	586			
2.43×10^{-7}	2.56	1317	1.83±0.077	705			

Table 11. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			26.0	793	RR[relative to $k(H_2)=9.62 \times 10^{-13}$]	Baldwin (1964)	
			1.36 ± 0.20	298 ± 1	FP-KS	Greiner (1967b)	
			7.79	753	RR[relative to $k(H_2)=7.87 \times 10^{-13}$]	Baker et al. (1970); Baldwin and Walker (1979)	
			1.21 ± 0.08	296	FP-KS	Greiner (1970)	296–497
			1.26 ± 0.14	298			
			1.19 ± 0.05	298			
			1.01 ± 0.04	299			
			1.10 ± 0.05	299			
			1.31 ± 0.02	299			
			1.30 ± 0.14	299			
			1.44 ± 0.04	335			
			1.91 ± 0.05	375			
			2.19 ± 0.07	423			
			2.92 ± 0.12	497			
			3.19 ± 0.15	497			
			3.16 ± 0.07	497			
			2.97 ± 0.15	497			
12.0		679 ± 39	3.39 ± 0.15	497			
			0.83 ± 0.17	300	DF-EPR/MS	Bradley et al. (1973)	
			2.22 ± 0.55	298	RR[relative to $k(CO)=1.55 \times 10^{-13}$]	Gorse and Volman (1974)	
			2.16 ± 0.10	381	PR-RA	Gordon and Mulac (1975)	381–416
			1.91 ± 0.09	416			
			5.23 ± 0.75	613	RR[relative to k(ethane) = $1.48 \times 10^{-17} T^2 e^{-499/T}$]	Hucknall et al. (1975)	613–653
			6.45 ± 0.83	653			
			1.98 ± 0.09	329 ± 5	MMS	Harker and Burton (1975)	
			2.02 ± 0.11	295 ± 2	FP-RA	Overend et al. (1975)	

Table 11. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.39 ± 0.20	300 ± 1	RR[relative to $k(n\text{-butane}) = 2.38 \times 10^{-12}$]	Darnall et al. (1978)	
			2.0	300	RR[relative to $k(\text{ethene}) = 8.44 \times 10^{-12}$][a]	Cox et al. (1980)	
			1.12 ± 0.04	299 ± 1	RR[relative to $k(n\text{-butane}) = 2.37 \times 10^{-12}$]	Atkinson et al. (1982b)	
			1.86 ± 0.15	428	RR[relative to $k(CO)=9.1\times 10^{-19}T^{1.77}e^{580/T}$]	Baulch et al. (1983)	428–696
			2.74 ± 0.24	489			
			2.82 ± 0.10	538			
			4.10 ± 0.22	589			
			4.95 ± 0.55	641			
			7.58 ± 0.72	696			
			1.05 ± 0.04	297	FP-RF	Tully et al. (1983)	297–690
			1.48 ± 0.06	326			
			2.51 ± 0.20	378			
			3.37 ± 0.23	469			
			4.78 ± 0.34	554			
1.59×10^{-3}	1.40	428	8.78 ± 0.97	690			
			26.2 ± 6.6	1220 ± 15	SH-RA	Bott and Cohen (1984)	
			1.0 ± 0.2	295	PLP-LIF	Schmidt et al. (1985)	
			1.20 ± 0.19	295 ± 2	DF-RA	Baulch et al. (1985)	
			21.9 ± 6.0	1074	LH-LIF	Smith et al. (1985)	
			1.10 ± 0.04	293	PLP-LIF	Droege and Tully (1986a)	293–854
			1.52 ± 0.06	342			
			1.61 ± 0.07	351.5			
			2.14 ± 0.09	401			
			2.49 ± 0.10	428			
			3.24 ± 0.13	491			
			3.36 ± 0.14	501.5			

Table 11. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.34 ± 0.14	505			
			4.84 ± 0.20	602			
			4.84 ± 0.20	603			
			7.28 ± 0.30	732			
1.04×10^{-4}	1.72	145	9.31 ± 0.38	854			
			1.05 ± 0.14	296.0 ± 1.1	RR[relative to k(*n*-butane) = 2.33×10^{-12}]	Edney et al. (1986)	
			1.28	300 ± 3	RR[relative to k(*n*-butane) = 2.38×10^{-12}]	Behnke et al. (1987)	
			1.27 ± 0.11	295 ± 2	PR-RA	Nielsen et al. (1988)	
			1.21 ± 0.10	297 ± 2	DF-LIF	Abbatt et al. (1990)	
			1.22 ± 0.08	298	PLP-RF	Mac Leod et al. (1990)	
			1.02 ± 0.05	298[b]	PLP-IR	Schiffman et al. (1991)	
			1.40 ± 0.30	298	PLP-RF	Dóbé et al. (1991)	
			0.996 ± 0.043	298 ± 2	RR[relative to k(2-methylpropane) = 2.12×10^{-12}]	Nielsen et al. (1991a)	
			1.07 ± 0.06	298	RR[relative to k(*n*-butane) = 2.36×10^{-12}]	Finlayson-Pitts et al. (1993)	
			1.07 ± 0.05	298			
			1.11 ± 0.04	298	RR[relative to k(2-methylpropane) = 2.12×10^{-12}]	Finlayson-Pitts et al. (1993)	
			1.05 ± 0.06	298			
			0.942 ± 0.095	298 ± 2	RR[relative to k(ethane) = 2.48×10^{-13}]	DeMore (1993c)	
			0.623 ± 0.016	233	PLP-LIF	Talukdar et al. (1994)	233–376
			0.741 ± 0.019	252			

Table 11. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.862 ± 0.023	272			
			1.123 ± 0.040	299			
			1.342 ± 0.064	325			
			1.574 ± 0.052	351			
1.58×10^{-5}	2	74 ± 25	1.816 ± 0.067	376			
10.1		657 ± 46					
			0.61 ± 0.04	233	PLP-LIF	Mellouki et al. (1994)	233–363
			0.75 ± 0.04	253			
			0.92 ± 0.04	273			
			1.05 ± 0.04	295			
			1.25 ± 0.04	318			
			1.51 ± 0.02	343			
9.81		650 ± 30	1.65 ± 0.07	363			
			1.09 ± 0.03	300	DF-LIF	Donahue et al. (1998)	299–394
			1.37 ± 0.04	325			
			1.46 ± 0.04	340			
			1.60 ± 0.09	360			
			1.85 ± 0.06	375			
			1.83 ± 0.10	390			
			0.3626 ± 0.0247	190	DF-LIF	Clarke et al. (1998)	190–360
			0.4136 ± 0.0127	200			
			0.4864 ± 0.0095	213			
			0.5602 ± 0.0063	225			
			0.6475 ± 0.0053	238			
			0.7532 ± 0.0051	250			
			0.8691 ± 0.0147	265			
			1.129 ± 0.0159	295			
			1.276 ± 0.0182	310			
			1.356 ± 0.0140	325			
			1.480 ± 0.0136	340			
			1.640 ± 0.0229	360			
			0.540	227	RR[relative to	DeMore and Bayes (1999)	227–428
			0.611	237	k(ethane) =		
			0.671	246	1.49×10^{-17}		
			0.808	265	$T^2 e^{-499/T}$]		
			0.878	273			
			0.961	283			
			0.999	287			
			1.09	298			

Table 11. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.35	323			
			1.52	343			
			1.62	349			
			1.96	383			
			2.52	428			
			1.15 ± 0.1	298	PLP-RF	Carl and Crowley (2001)	
			1.17 ± 0.1	298			
			0.46 ± 0.02	210	FP-RF	Kozlov et al. (2003)	210–480
			0.539 ± 0.007	220			
			0.579 ± 0.009	230			
			0.732 ± 0.012	250			
			0.884 ± 0.016	272			
			1.13 ± 0.02	298			
			1.43 ± 0.03	330			
			1.86 ± 0.05	370			
			2.43 ± 0.04	420			
5.81×10^{-5}	1.83	167	3.34 ± 0.07	480			

[a] From Atkinson (1997).
[b] Room temperature; assumed to be ~298 K.

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Table 12. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane-d_2 [$CH_3CD_2CH_3$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.610±0.028	295	PLP-LIF	Droege and Tully (1986a)	295–854
			0.802±0.034	328.5			
			1.20±0.05	376.5			
			1.72±0.07	437.2			
			2.47±0.10	503.5			
			3.79±0.16	603			
			5.92±0.24	732			
2.02×10^{-4}	1.63	383	7.86±0.32	854			

Table 13. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane-d_3 [$CH_3CH_2CD_3$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.984±0.050	295	PLP-LIF	Droege and Tully (1986a)	295–854
			1.28±0.06	328.5			
			1.62±0.07	376.5			
			2.17±0.09	437.2			
			2.88±0.12	503.5			
			4.19±0.18	603			
			6.20±0.26	728			
2.26×10^{-5}	1.90	40	8.06±0.34	854			

Table 14. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane-d_5 [$CH_3CD_2CD_3$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.478±0.021	295	PLP-LIF	Droege and Tully (1986a)	295–840
			0.621±0.026	328.5			
			0.950±0.040	376.5			
			1.38±0.06	437.2			
			1.96±0.08	503.5			
			3.13±0.13	603			
			4.93±0.20	728			
2.59×10^{-5}	1.91	303	6.60±0.27	840			

Table 15. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane-d_6 [$CD_3CH_2CD_3$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.826±0.040	295	PLP-LIF	Droege and Tully (1986a)	295–840
			0.999±0.045	328.5			
			1.37±0.06	376.5			
			1.79±0.08	437.2			
			2.46±0.10	503.5			
			3.55±0.15	603			
			5.31±0.22	732			
1.03×10^{-5}	2.00	23	6.78±0.28	840			

Table 16. Rate constants and temperature-dependent parameters for the reaction of OH radicals with propane-d_8 [$CD_3CD_2CD_3$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.408±0.045	295	PLP-LIF	Droege and Tully (1986a)	295–854
			0.527±0.043	328.5			
			0.746±0.047	376.5			
			1.09±0.06	437.2			
			1.50±0.07	503.5			
			2.55±0.11	603			
			4.25±0.18	728			
2.36×10^{-7}	2.53	15	5.88±0.25	854			

Table 17. Rate constants and temperature-dependent parameters for the reaction of OH radicals with *n*-butane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			34.6	793	RR [relative to $k(H_2)$=9.62 × 10^{-13}]	Baldwin and Walker (1964)	
			10.4	753	RR [relative to $k(H_2)$=7.87 × 10^{-13}]	Baker et al. (1970); Baldwin and Walker (1979)	
			2.56 ± 0.09	298	FP-KS	Greiner (1970)	298–495
			2.59 ± 0.22	301			
			2.79 ± 0.32	336			
			2.96 ± 0.10	373			
			4.85 ± 0.19	425			
			4.12 ± 0.15	428			
14.1		524 ± 94	4.90 ± 0.17	495			
			4.1	298	RR [relative to k(propene, 1 Torr He) = 1.7×10^{-11}][a]	Morris and Niki (1971)	
			2.35 ± 0.35	298	FP-RF	Stuhl (1973)	
			3.01 ± 0.76	298	RR [relative to k(CO)=1.55 × 10^{-13}]	Gorse and Volman (1974)	
			4.22 ± 0.17	298	PR-RA	Gordon and Mulac (1975)	298–416
			4.15 ± 0.17	381			
			4.98 ± 0.17	416			
			9.49 ± 0.80	653	RR [relative to k(propane) = 6.16×10^{-12}]	Hucknall et al. (1975)	
			2.46 ± 0.15	292 ± 2	RR [relative to k(CO)=1.66 × 10^{-13}]	Campbell et al. (1975)	
			2.72 ± 0.27	297.7	FP-RF	Perry et al. (1976)	297–420
			3.54 ± 0.35	351.0			
17.6		559 ± 151	4.69 ± 0.47	419.6			

Table 17. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			2.67 ± 0.22	297 ± 2	FP-RA	Paraskevopoulos and Nip (1980)	
			2.52 ± 0.25	299 ± 2	RR [relative to k(propene) = 2.62×10^{-11}][b]	Atkinson et al. (1981)	
			2.71 ± 0.33	295 ± 1	RR [relative to k(propene) = 2.68×10^{-11}][b]	Atkinson and Aschmann (1984)	
			2.3 ± 0.3	295	PLP-LIF	Schmidt et al. (1985)	
			2.42 ± 0.10 2.95 ± 0.12 3.53 ± 0.15 4.56 ± 0.19	294 332 377 439	PLP-LIF	Droege and Tully (1986b)	294–509
2.34×10^{-5}	1.95	−134	5.84 ± 0.25	509			
			2.70 ± 0.34	300	RR [relative to k(ethene) = 8.44×10^{-12}][b]	Barnes et al. (1986)	
			2.36 ± 0.04	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)	
			2.25 ± 0.10	297 ± 2	DF-LIF	Abbatt et al. (1990)	
			2.32 ± 0.08	~298[c]	PLP-IR	Schiffman et al. (1991)	
			1.560 ± 0.015 1.788 ± 0.018 2.097 ± 0.024 2.459 ± 0.018 2.828 ± 0.060 3.196 ± 0.032	231 252 273 299 328 352	PLP-LIF	Talukdar et al. (1994)	231–378
2.04×10^{-5} 11.8	2	−85 ± 8 470 ± 40 (231–298 K)	3.647 ± 0.022	378			

Table 17. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			2.43 ± 0.07	300	DF-LIF	Donahue et al. (1998)	299–386
			2.74 ± 0.08	325			
			2.87 ± 0.09	340			
			3.48 ± 0.10	375			
			3.54 ± 0.11	390			
			1.52	235	RR [relative to	DeMore and Bayes (1999)	235–361
			1.73	251	k(propane) =		
			1.90	264	1.65×10^{-17}		
			1.96	275	$T^2 e^{-87/T}$]		
			2.24	293			
			2.33	298			
			2.70	328			
			2.96	336			
			3.24	358			
			3.32	361			
			2.6 ± 0.5	300	DF-LIF	Chuong and Stevens (2002)	
			2.6 ± 0.2	300			

[a] Measured under the same conditions by Morris et al. (1971).
[b] From Atkinson (1997).
[c] Room temperature; assumed to be ~298 K.

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Table 18. Rate constants and temperature-dependent parameters for the reaction of OH radicals with *n*-butane-d_{10}

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.697±0.0069	297±2	FP-RA	Paraskevopoulov and Nip (1980)	
			0.893±0.037	294	PLP-LIF	Droege and Tully (1986b)	294–599
			1.13±0.05	332			
			1.49±0.06	377			
			2.07±0.09	439			
			2.87±0.12	509			
2.92×10^{-6}	2.20	−33	3.98±0.17	599			

Table 19. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2-methylpropane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			19.2	793	RR [relative to $k(H_2)=9.62 \times 10^{-13}$]	Baldwin and Walker (1964)	
			2.13 ± 0.12	297 ± 1	FP-KS	Greiner (1967b)	
			9.92	753	RR [relative to $k(H_2)=7.87 \times 10^{-13}$]	Baker et al. (1970); Baldwin and Walker (1979)	
			2.14 ± 0.12	297	FP-KS	Greiner (1970)	297–498
			2.23 ± 0.05	297			
			2.67 ± 0.17	298			
			2.56 ± 0.05	304			
			2.69 ± 0.15	305			
			3.01 ± 0.07	338			
			2.91 ± 0.07	371			
			3.04 ± 0.14	374			
			3.57 ± 0.15	425			
8.7		387 ± 63	4.25 ± 0.22	498			
			3.64 ± 0.91	298	RR [relative to $k(CO)=1.55 \times 10^{-13}$]	Gorse and Volman (1972/73); Gorse and Volman (1974)	
			7.88 ± 0.44	653	RR [relative to k(propane) = 6.16×10^{-12}]	Hucknall et al. (1975)	
			2.2	303	RR [relative to $k(cis$-2-butene) = 5.49×10^{-11}][a]	Wu et al. (1976)	
			2.20 ± 0.05	300 ± 1	RR [relative to $k(n$-butane) = 2.38×10^{-12}]	Darnall et al. (1978)	
			2.70 ± 0.22	267	PLP-RF	Trevor et al. (1982)	267–324
			3.6	298			
			3.62 ± 0.40	324			
			2.07 ± 0.05	297 ± 2	RR [relative to $k(n$-butane) = 2.34×10^{-12}]	Atkinson et al. (1984)	

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Table 19. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.83 ± 0.34	296	PLP-LMR	Böhland et al. (1984)	
			1.9 ± 0.3	295	PLP-LIF	Schmidt et al. (1985)	
			2.19 ± 0.11	293	PLP-LIF	Tully et al. (1986b)	293–864
			2.59 ± 0.13	342			
			3.21 ± 0.16	403			
			3.49 ± 0.17	424			
			4.03 ± 0.20	470			
			4.58 ± 0.23	509.5			
			5.49 ± 0.27	574			
			7.40 ± 0.37	705			
4.31×10^{-5}	1.80	−175	10.13 ± 0.51	864			
			2.18 ± 0.31	297.8 ± 0.4	RR [relative to k(*n*-butane) = 2.35×10^{-12}]	Edney et al. (1986)	
			20.9 ± 4.2	1146 ± 15	SH-RA	Bott and Cohen (1989)	
			2.11 ± 0.09	~298[b]	PLP-IR	Schiffman et al. (1991)	
			1.55 ± 0.18	213	PLP-LIF	Talukdar et al. (1994)	213–372
			1.58 ± 0.09	224			
			1.69 ± 0.06	234			
			1.67 ± 0.06	243			
			1.745 ± 0.06	253			
			1.82 ± 0.11	272			
			2.13 ± 0.10	296			
			2.19 ± 0.04	297			
			1.96 ± 0.09	298			
			2.29 ± 0.07	323			
			2.40 ± 0.10	343			
			2.54 ± 0.03	357			
9.32×10^{-6} 5.72	2	−274 ± 16 293 ± 40 (213–298 K)	2.73 ± 0.06	372			

Table 19. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			2.09 ± 0.06	300	DF-LIF	Donahue et al. (1998)	298–388
			2.38 ± 0.07	325			
			2.47 ± 0.09	340			
			2.62 ± 0.08	375			
			2.72 ± 0.14	390			

[a] From Atkinson (1997).
[b] Room temperature; assumed to be ~298 K.

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Table 20. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2-methylpropane-d_1 [$(CH_3)_3CD$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.36±0.07	293.5	PLP-LIF	Tully et al. (1986b)	293–864
			1.81±0.09	344			
			2.44±0.12	403			
			3.35±0.17	473			
			4.84±0.24	574			
			7.12±0.36	705			
1.20×10^{-4}	1.69	85	9.90±0.49	864			

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Table 21. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2-methylpropane-d_9 [$(CD_3)_3CH$]

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.70±0.09	293.5	PLP-LIF	Tully et al. (1986b)	293–864
			1.91±0.10	343			
			2.27±0.11	403			
			2.81±0.14	471			
			3.64±0.18	574			
			5.28±0.26	705			
1.08×10^{-7}	2.57	−569	7.61±0.38	864			

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Table 22. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2-methylpropane-d_{10} [$(CD_3)_3CD$]

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.956±0.067	293.5	PLP-LIF	Tully et al. (1986b)	293–864
			1.21±0.08	340.5			
			1.58±0.09	403			
			2.10±0.12	473			
			3.09±0.15	574			
			4.92±0.25	705			
9.12×10^{-8}	2.63	−352	7.30±0.37	864			

Table 23. Rate constants and temperature-dependent parameters for the reaction of OH radicals with *n*-pentane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			6.6	303	RR [relative to $k(cis$-2-butene) = 5.49×10^{-11}][a]	Wu et al. (1976)	
			3.26 ± 0.12	300 ± 1	RR [relative to $k(n$-butane) = 2.38×10^{-12}]	Darnall et al. (1978)	
			14.2	753	RR [relative to $k(H_2)$=7.87 × 10^{-13}]	Baldwin and Walker (1979)	
			5.3	300	RR [relative to k(ethene) = 8.44×10^{-12}][a]	Cox et al. (1980)	
			4.1	300	RR [relative to k(ethene) = 8.44×10^{-12}][a]	Barnes et al. (1982)	
			3.78 ± 0.05	299 ± 2	RR [relative to $k(n$-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982b)	
			3.87	300 ± 3	RR [relative to $k(n$-butane) = 2.38×10^{-12}]	Behnke et al. (1987)	
			3.98 ± 0.15	312	RR [relative to $k(n$-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)	
			2.49 ± 0.32 2.60 ± 0.21 3.02 ± 0.29 3.67 ± 0.17 3.97 ± 0.37 4.40 ± 0.20	243 263 273 298 314 325	RR [relative to k(2-methylpropane) = 1.17×10^{-17} $T^2 e^{213/T}$]	Harris and Kerr (1988)	243–325

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Table 23. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.15 ± 0.72	247	RR [relative to k(*n*-butane) = $1.81 \times 10^{-17} T^2 e^{114/T}$]	Harris and Kerr (1988)	247–327
			2.78 ± 0.33	253			
			2.91 ± 0.26	263			
			3.05 ± 0.19	273			
			3.27 ± 0.25	275			
			3.30 ± 0.20	282			
			3.94 ± 0.14	295			
			3.94 ± 0.35	305			
			3.78 ± 0.34	314			
			4.27 ± 0.11	325			
			4.19 ± 0.33	327			
			3.83 ± 0.05	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)	
			4.21 ± 0.18	297 ± 2	DF-LIF	Abbatt et al. (1990)	
			3.87 ± 0.05	302	RR [relative to k(2-methylpropane) = 2.16×10^{-12}]	Donaghy et al. (1993)	
			2.64 ± 0.06	224	PLP-LIF	Talukdar et al. (1994)	224–372
			2.67 ± 0.14	233			
			2.75 ± 0.10	233			
			2.85 ± 0.10	233			
			3.11 ± 0.09	253			
			3.54 ± 0.11	272			
			4.02 ± 0.20	296			
			4.01 ± 0.11	297			
			4.04 ± 0.10	297			
			4.50 ± 0.12	309			
			4.83 ± 0.08	323			
			5.06 ± 0.12	340			
			5.54 ± 0.26	358			
3.13×10^{-5} 15.0	2	−116 ± 24 392 ± 40 (224–297 K)	5.81 ± 0.16	372			

Table 23. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.98 ± 0.13	300	DF-LIF	Donahue et al. (1998)	299–407
			4.68 ± 0.33	325			
			4.59 ± 0.18	340			
			5.47 ± 0.16	360			
			5.83 ± 0.44	375			
			6.44 ± 0.37	390			
			3.76	308	RR [relative to k(propane) = $1.65 \times 10^{-17} T^2 e^{-87/T}$]	DeMore and Bayes (1999)	308–345
			4.50	345			
			2.74	233	RR [relative to k(n-butane) = $1.81 \times 10^{-17} T^2 e^{114/T}$]	DeMore and Bayes (1999)	233–364
			3.00	253			
			3.25	273			
			3.71	298			
			4.15	326			
			4.63	351			
			4.92	364			

[a] From Atkinson (1997).

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Table 24. Rate constants for the reaction of OH radicals with 2-methylbutane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
2.70±0.54	305±2	RR[relative to k(*n*-butane) = 2.45×10^{-12}]	Lloyd et al. (1976)
3.30±0.07	300±1	RR[relative to k(*n*-butane) = 2.38×10^{-12}]	Darnall et al. (1978)
3.7	300	RR[relative to k(ethene) = 8.44×10^{-12}][a]	Cox et al. (1980)
3.60±0.10	297±2	RR[relative to k(*n*-butane) = 2.34×10^{-12}]	Atkinson et al. (1984)

[a] from Atkinson (1997).

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Table 25. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,2-dimethylpropane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.741 ± 0.020	292	FP-KS	Greiner (1970)	292–493
			0.859 ± 0.039	292			
			0.875 ± 0.025	298			
			1.16 ± 0.08	335			
			1.41 ± 0.04	370			
			2.11 ± 0.10	424			
14.1		844 ± 45	2.54 ± 0.09	493			
			13.1 ± 2.4	753	RR [relative to $k(H_2) = 7.87 \times 10^{-13}$]	Baker et al. (1970)	
			8.03	753	RR [relative to $k(H_2) = 7.87 \times 10^{-13}$]	Baker et al. (1976); Baldwin and Walker (1979)	
			0.91 ± 0.15	300 ± 1	RR [relative to k(*n*-butane) = 2.38×10^{-12}]	Darnall et al. (1978)	
			0.910 ± 0.10	297 ± 2	FP-RA	Paraskevopoulos and Nip (1980)	
			0.705 ± 0.037	299 ± 2	RR [relative to k(*n*-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982a)	
			0.909 ± 0.115	287	PLP-LIF	Tully et al. (1985, 1986a)	287–901
			1.27 ± 0.14	350			
			2.08 ± 0.19	431			
			3.17 ± 0.25	518			
			4.46 ± 0.38	600			
			7.02 ± 0.67	705			
			10.1 ± 1.1	812			
8.60×10^{-9}	3.05	−340	12.5 ± 1.5	901			
			0.79 ± 0.10	298 ± 2	PR-RA	Nielsen et al. (1991b)	
			0.78 ± 0.10	298 ± 2	RR [relative to k(*n*-butane) = 2.36×10^{-12}]	Nielsen et al. (1991b)	

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Table 26. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,2-dimethylpropane-d_{12}

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.180 ± 0.012	290	PLP-LIF	Tully et al. (1985, 1986a)	290–903
			0.375 ± 0.025	352			
			0.728 ± 0.048	430			
			1.30 ± 0.09	508.5			
			2.19 ± 0.17	598			
			3.94 ± 0.34	705			
			5.62 ± 0.55	812			
1.08×10^{-7}	2.71	307	8.09 ± 0.89	903			

Table 27. Rate constants for the reaction of OH radicals with *n*-hexane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
5.1±1.1	305±2	RR [relative to k(*n*-butane) = 2.45 × 10^{-12}]	Lloyd et al. (1976)	
6.0	303	RR [relative to k(*cis*-2-butene) = 5.49 × 10^{-11}][a]	Wu et al. (1976)	
5.6±0.8	292	RR [relative to k(*n*-butane) = 2.28 × 10^{-12}]	Campbell et al. (1976)	
5.23±0.09	299±2	RR [relative to k(*n*-butane) = 2.37 × 10^{-12}]	Atkinson et al. (1982a)	
5.55±0.20	298±2	RR [relative to k(propene) = 2.63 × 10^{-11}][a]	Atkinson et al. (1983a)	
5.31±0.46	295±1	RR [relative to k(propene) = 2.68 × 10^{-11}][a]	Atkinson and Aschmann (1984)	
5.17±0.52	295	RR [relative to k(*n*-butane) = 2.32 × 10^{-12}]	Klein et al. (1984)	
6.2	300	RR [relative to k(toluene) = 5.58 × 10^{-12}][b]	Klöpffer et al. (1986)	
5.91±0.68	300±2	RR [relative to k(ethene) = 8.44 × 10^{-12}][a]	Barnes et al. (1986)	
5.20	300±3	RR [relative to k(*n*-butane) = 2.38 × 10^{-12}]	Behnke et al. (1987)	
5.75±0.56	312	RR [relative to k(*n*-heptane) = 6.97 × 10^{-12}]	Nolting et al. (1988)	
5.27±0.04	300	RR [relative to k(*n*-octane) = 8.15 × 10^{-12}]	Behnke et al. (1988)	
5.37±0.20	301±2	RR [relative to k(*n*-pentane) = 3.86 × 10^{-12}]	McLoughlin et al. (1993)	
21.8	962±16	SH-RA	Koffend and Cohen (1996)	
5.45±0.16 6.11±0.18 6.23±0.19 6.43±0.45 7.33±0.62 7.29±0.22	300 325 340 360 375 390	DF-LIF	Donahue et al. (1998)	298–393

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Table 27. Continued

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Temperature Reference	Range (K)
5.07	292	RR [relative to k(propane) = $1.65 \times 10^{-17} T^2 e^{-87/T}$]	DeMore and Bayes (1999)	292–366
5.12	298			
5.46	307			
5.73	315			
5.74	321			
6.22	337			
5.97	339			
6.84	353			
6.67	357			
7.37	366			
5.00	294	RR [relative to k(n-butane) = $1.81 \times 10^{-17} T^2 e^{114/T}$]	DeMore and Bayes (1999)	294–367
5.31	310			
5.65	329			
6.33	354			
6.62	367			
5.41	303	RR [relative to k(n-pentane) = 3.90×10^{-12}]	DeMore and Bayes (1999)	

[a] From Atkinson (1997).
[b] From Calvert et al. (2002).

Table 28. Rate constants for the reaction of OH radicals with 2-methylpentane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
4.34 ± 0.87	305 ± 2	RR[relative to k(*n*-butane) = 2.45 × 10^{-12}]	Lloyd et al. (1976)
5.3	300	RR[relative to k(ethene) = 8.44 × 10^{-12}][a]	Cox et al. (1980)
5.15 ± 0.22	297 ± 2	RR[relative to k(*n*-butane) = 2.34 × 10^{-12}]	Atkinson et al. (1984)

[a] From Atkinson (1997).

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Table 29. Rate constants for the reaction of OH radicals with 3-methylpentane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
5.9±1.2	305±2	RR[relative to $k(n\text{-butane}) = 2.45 \times 10^{-12}$]	Lloyd et al. (1976)
5.24±0.10	297±2	RR[relative to $k(n\text{-butane}) = 2.34 \times 10^{-12}$]	Atkinson et al. (1984)

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Table 30. Rate constants for the reaction of OH radicals with 2,2-dimethylbutane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
2.41±0.08	297±2	RR[relative to $k(n\text{-butane}) = 2.34 \times 10^{-12}$]	Atkinson et al. (1984)	
1.18±0.24	245	RR[relative to $k(n\text{-pentane}) = 2.52 \times 10^{-17} T^2 e^{158/T}$]	Harris and Kerr (1988)	245–328
1.36±0.18	247			
1.33±0.25	253			
1.58±0.20	263			
1.82±0.34	273			
1.80±0.29	283			
2.14±0.35	299			
2.22±0.32	303			
2.37±0.24	303			
2.56±0.25	313			
2.91±0.44	326			
2.79±0.27	328			

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Table 31. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,3-dimethylbutane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			7.46±0.22	300	FP-KS	Greiner (1970)	300–498
			6.71±0.22	336			
			6.81±0.35	372			
			7.11±0.65	424			
4.79		−129±67	5.94±1.25	498			
			4.94±0.99	305±2	RR [relative to k(2-methylpropene) = 4.94 × 10^{-11}][a]	Darnall et al. (1976)	
			4.94±0.26	300±1	RR [relative to k(*n*-butane) = 2.38 × 10^{-12}]	Darnall et al. (1978)	
			4.0	300	RR [relative to k(ethene) = 8.44 × 10^{-12}]a	Cox et al. (1980)	
			5.79±0.03	299±2	RR [relative to k(cyclohexane) = 7.00 × 10^{-12}]	Atkinson et al. (1982a)	

Table 31. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			6.11±1.05	247	RR [relative	Harris and Kerr (1988)	247–327
			5.02±1.08	253	to k(*n*-butane)		
			5.40±0.62	263	$= 1.81 \times 10^{-17}$		
			5.19±0.87	273	$T^2 e^{114/T}$]		
			5.22±1.06	275			
			5.29±0.33	282			
			5.48±0.21	295			
			5.56±0.40	305			
			4.65±0.72	314			
			5.68±0.11	325			
			5.45±0.50	327			
			5.56±0.38	247	RR [relative to	Harris and Kerr (1988)	247–327
			5.15±0.82	253	k(*n*-pentane) =		
			5.53±1.05	263	2.52×10^{-17}		
			5.29±0.41	273	$T^2 e^{158/T}$]		
			5.46±0.85	275			
			5.48±0.53	282			
			5.21±0.15	295			
			5.71±0.12	305			
			5.22±0.50	314			
			5.76±0.09	325			
			5.68±0.18	327			
			34.5±5.2	1220±16	SH-RA	Bott and Cohen (1991b)	

[a] From Atkinson (1997).

Table 32. Rate constants for the reaction of OH radicals with *n*-heptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
6.68 ± 0.11	299 ± 2	RR [relative to k(*n*-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982b)
7.8	300	RR [relative to k(toluene) = 5.58×10^{-12}][a]	Klöpffer et al. (1986)
6.60	300 ± 3	RR [relative to k(*n*-butane) = 2.38×10^{-12}]	Behnke et al. (1987)
6.78 ± 0.08	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)
33.4	1086 ± 16	SH-RA	Koffend and Cohen (1996)
6.97 ± 0.29	295 ± 2	RR [relative to k(*n*-octane) = 8.05×10^{-12}]	Ferrari et al. (1996)

[a] From Calvert et al. (2002).

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Table 33. Rate constants for the reaction of OH radicals with 2,4-dimethylpentane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
4.77±0.10	297±2	RR [relative to $k(n\text{-butane}) = 2.34 \times 10^{-10}$]	Atkinson et al. (1984)

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Table 34. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,2,3-trimethylbutane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			5.23 ± 0.12	296	FP-KS	Greiner (1970)	296–497
			4.87 ± 0.12	303			
			4.50 ± 0.34	371			
			4.60 ± 0.27	373			
7.95		115 ± 73	6.33 ± 0.19	497			
			3.66 ± 0.74	305 ± 2	RR [relative to k(2-methylpropene) = 4.94×10^{-11}][a]	Darnall et al. (1976)	
			9.6 ± 1.2	753	RR [relative to $k(H_2)=7.87 \times 10^{-13}$]	Baldwin et al. (1981)	
			3.81 ± 0.08	297 ± 2	RR [relative to k(*n*-butane) = 2.34×10^{-12}]	Atkinson et al. (1984)	
			3.02 ± 0.45	263	RR [relative to k(*n*-pentane) = $2.52 \times 10^{-17} T^2 e^{158/T}$]	Harris and Kerr (1988)	263–303
			4.13 ± 0.39	283			
			4.06 ± 0.24	303			
			3.90 ± 0.55	303			
			2.97 ± 0.98	263	RR [relative to k(2,2-dimethylbutane) = $3.37 \times 10^{-11} e^{-809/T}$]	Harris and Kerr (1988)	263–303
			2.32 ± 1.16	283			
			4.60 ± 0.85	303			
			4.57 ± 1.02	303			

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Table 34. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.73 ± 0.51	243	RR [relative to	Harris and Kerr (1988)	243–324
			3.55 ± 0.22	244	$k(n$-hexane) =		
			3.48 ± 0.34	253	2.54×10^{-14}		
			3.81 ± 0.47	263	$Te^{-112/T}$]		
			3.76 ± 0.68	273			
			3.86 ± 0.54	282			
			3.87 ± 0.18	295			
			3.85 ± 0.19	314			
			3.98 ± 0.49	324			
			3.84 ± 0.15	324			

[a] From Atkinson (1997).

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Table 35. Rate constants and temperature-dependent parameters for the reaction of OH radicals with *n*-octane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			8.42±1.25	296	FP-KS	Greiner (1970)	296–497
			12.0±0.7	371			
			10.8±0.5	371			
29.5		364±61	14.3±0.4	497			
			8.25±0.11	299±2	RR [relative to k(*n*-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982b)	
			8.03	300±3	RR [relative to k(*n*-butane) = 2.38×10^{-12}]	Behnke et al. (1987)	
			8.16±0.28	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)	
			44.2	1078±16	SH-RA	Koffend and Cohen (1996)	

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Table 36. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,2,4-trimethylpentane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			3.90±0.15	298	FP-KS	Greiner (1970)	298–493
			3.55±0.12	305			
			4.37±0.24	339			
			5.25±0.15	373			
			5.43±0.14	423			
15.5		426±64	6.63±0.42	493			
			3.32±0.15	297±2	RR [relative to $k(n$-butane) = 2.34×10^{-12}]	Atkinson et al. (1984)	
			37.2±5.6	1186±16	SH-RA	Bott and Cohen (1991b)	

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Table 37. Rate constants for the reaction of OH radicals with 2,3,4-trimethylpentane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
7.78±0.20	243	RR[relative to k(*n*-hexane) = $2.54 \times 10^{-14} T e^{-112/T}$]	Harris and Kerr (1988)	243–313
7.85±0.83	253			
6.63±0.40	263			
6.95±0.37	273			
6.46±0.21	295			
6.49±0.11	303			
6.62±0.56	313			
7.23±0.17	313			

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Table 38. Rate constants and temperature-dependent parameters for the reaction of OH radicals with 2,2,3,3-tetramethylbutane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.08±0.02	294	FP-KS	Greiner (1970)	294-495
			1.16±0.11	301			
			1.42±0.04	335			
			2.04±0.09	370			
			2.21±0.07	424			
16.2		802±63	3.52±0.12	495			
			6.30±0.79	753	RR [relative to $k(H_2) = 7.87 \times 10^{-13}$]	Baldwin et al. (1979); Baldwin and Walker (1979)	
			0.959±0.071	297±2	RR [relative to $k(n\text{-butane}) = 2.34 \times 10^{-12}$]	Atkinson et al. (1984)	
			0.948±0.020	290	PLP-LIF	Tully et al. (1985)	290–738
			1.48±0.04	348.5			
			2.38±0.03	423.5			
			3.58±0.05	506			
			5.27±0.09	606			
4.75×10^{-6}	2.20	68	9.36±0.35	737.5			
			29.9±4.5	1180±16	SH-RA	Bott and Cohen (1991b)	

Table 39. Rate constants for the reaction of OH radicals with *n*-nonane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
9.76±0.27	299±2	RR [relative to k(*n*-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982b)
9.69	300±3	RR [relative to k(*n*-butane) = 2.38×10^{-12}]	Behnke et al. (1987)
9.45±0.28	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)
9.55±0.19	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)
45.5	1097±16	SH-RA	Koffend and Cohen (1996)
9.72±0.22	295±2	RR [relative to k(*n*-octane) = 8.05×10^{-12}]	Ferrari et al. (1996)
10.3±0.3	296±2	RR [relative to k(propene) = 2.66×10^{-11}][a]	Kramp and Paulson (1998)
9.16±1.2[b]	295±2	RR [relative to k(*n*-octane) = 8.05×10^{-12}]	Coeur et al. (1998, 1999)

[a] From Atkinson (1997).
[b] Two standard deviation uncertainty estimated from the data given (Coeur et al., 1998, 1999); could be larger, at ±2.1.

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Table 40. Rate constants for the reaction of OH radicals with 3,3-diethylpentane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
5.1±0.8	298±2	PR-RA	Nielsen et al. (1991b)
4.46±0.28	298±2	RR [relative to k(cyclohexane) = 6.97×10^{-12}]	Nielsen et al. (1991b)

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Table 41. Rate constants for the reaction of OH radicals with *n*-decane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
10.4±0.5	299±2	RR [relative to k(*n*-hexane) = 5.22×10^{-12}]	Atkinson et al. (1982b)
10.8±0.4	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)
11.5±0.2	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)
56.4	1109±16	SH-RA	Koffend and Cohen (1996)
11.6±0.4	296±2	RR [relative to k(*n*-octane) = 8.07×10^{-12}]	Aschmann et al. (2001)

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Table 42. Rate constants for the reaction of OH radicals with 3,4-diethylhexane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
6.92± 0.45	296 ± 2	RR [relkative to k(*n*-octane) = 8.07 × 10^{-12}]	Aschmann et al. (2001)

Table 43. Rate constants for the reaction of OH radicals with *n*-undecane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
12.7±0.3	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)
12.3 ± 0.2	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)

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Table 44. Rate constants for the reaction of OH radicals with *n*-dodecane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
14.0±0.5	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)
12.9±0.2	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)

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Table 45. Rate constants for the reaction of OH radicals with *n*-tridecane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
16.2±0.6	312	RR [relative to k(*n*-heptane) = 6.97×10^{-12}]	Nolting et al. (1988)
14.4±0.2	300	RR [relative to k(*n*-octane) = 8.15×10^{-12}]	Behnke et al. (1988)

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Table 46. Rate constants for the reaction of OH radicals with *n*-tetradecane

$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference
17.9±0.7	312	RR [relative to k(*n*-heptane) = 6.97 × 10^{-12}]	Nolting et al. (1988)

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Table 47. Rate constants for the reaction of OH radicals with *n*-pentadecane

$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference
20.7±1.0	312	RR [relative to k(*n*-heptane) = 6.97 × 10^{-12}]	Nolting et al. (1988)

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Table 48. Rate constants for the reaction of OH radicals with *n*-hexadecane

$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference
23.2±1.3	312	RR [relative to k(*n*-heptane) = 6.97 × 10^{-12}]	Nolting et al. (1988)

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Table 49. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclopropane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0621 ± 0.0138	298 ± 2	FP-RA	Jolly et al. (1985)	
			0.111 ± 0.024	298 ± 3	PLP-RF	Dóbé et al. (1991, 1992)	298–492
			0.133 ± 0.008	325 ± 1			
			0.152 ± 0.022	337 ± 1			
			0.191 ± 0.042	362 ± 1			
			0.236 ± 0.016	388 ± 1			
			0.365 ± 0.058	467 ± 2			
			0.412 ± 0.034	476 ± 3			
3.9		1107 ± 51	0.462 ± 0.062	492 ± 3			
1.17×10^{-4}	1.5	522 ± 44					
			0.0212 ± 0.0043	200	DF-LIF	Clarke et al. (1998)	200–360
			0.0296 ± 0.0017	213			
			0.0347 ± 0.0004	225			
			0.0378 ± 0.0004	238			
			0.0426 ± 0.0004	250			
			0.0515 ± 0.0013	265			
			0.0591 ± 0.0007	280			
			0.0657 ± 0.0008	295			
			0.0752 ± 0.0012	310			
			0.0897 ± 0.0024	325			
			0.1009 ± 0.0002	340			
			0.1161 ± 0.0075	360			
			0.0538	276	RR [relative to k(ethane) = $1.49 \times 10^{-17} T^2 e^{-499/T}$]	DeMore and Bayes (1999)	276–421
			0.0742	298			
			0.0765	300			
			0.0952	316			
			0.140	348			
			0.167	363			
			0.198	383			
			0.243	403			
			0.285	421			

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Table 49. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			0.0751 ± 0.0025	298.3 ± 0.1	RR [relative to	Wilson et al. (2001)	298–459
			0.0769 ± 0.0010	298.3 ± 0.1	k(ethane) =		
			0.108 ± 0.001	323.4 ± 0.2	1.49×10^{-17}		
			0.189 ± 0.003	373.1 ± 0.3	$T^2 e^{-499/T}$]		
			0.260 ± 0.003	401.3 ± 2			
			0.300 ± 0.003	415.6 ± 2			
			0.381 ± 0.008	444.9 ± 2			
			0.427 ± 0.003	458.7 ± 2			
			0.0571 ± 0.0003	271.5 ± 0.3	RR [relative to	Wilson et al. (2001)	271–463
			0.0634 ± 0.0030	278.3 ± 0.1	$k(CH_3CHF_2)$=		
			0.0797 ± 0.0008	298.2 ± 0.1	1.98×10^{-18}		
			0.0885 ± 0.0009	304.3 ± 0.0	$T^2 e^{-460/T}$][a]		
			0.110 ± 0.004	324.5 ± 0.2			
			0.148 ± 0.004	348.7 ± 0.2			
			0.184 ± 0.003	372.7 ± 0.2			
			0.237 ± 0.005	399.3 ± 0.2			
			0.262 ± 0.011	408.2 ± 2			
			0.297 ± 0.009	424.7 ± 2			
			0.341 ± 0.015	446.6 ± 2			
			0.407 ± 0.016	463.4 ± 1.3			

[a] From the IUPAC evaluation (IUPAC, 2003)

Table 50. Rate constants for the reaction of OH radicals with isopropylcyclopropane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
2.61± 0.05	296±2	RR [relative to k(*n*-butane) = 2.33×10^{-12}]	Atkinson and Aschmann (1988)

Table 51. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclobutane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.2±0.3	298	RR [relative to k(CO) = 1.55 × 10^{-13}]	Gorse and Volman (1974)	
			1.75±0.15	298	PLP-RF	Dóbé et al. (1991)	
			1.75±0.12	298±3	PLP-RF	Dóbé et al. (1992)	298–469
			2.22±0.20	327±1			
			2.36±0.14	360±2			
			2.89±0.30	392±2			
			3.49±0.28	429±2			
5.06×10^{-4}	1.5	115±40	3.98±0.40	469±3			
			1.74	272	RR [relative to k(propane) = 1.65×10^{-17} $T^2 e^{-87/T}$]	DeMore and Bayes (1999)	272–366
			1.93	288			
			1.95	293			
			1.90	298			
			2.11	303			
			2.24	309			
			2.63	343			
			3.06	366			

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Table 52. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclopentane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			6.3	298	RR [relative to k(CO) = 1.55×10^{-13}]	Volman (1975)	
			4.11±0.25	300±1	RR [relative to k(*n*-butane) = 2.38×10^{-12}]	Darnall et al. (1978)	
			4.93±0.05	299±2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1982a)	
			5.18±0.38	298±2	FP-RA	Jolly et al. (1985)	
			5.02±0.22 6.12±0.27 7.23±0.32	295 344 402.5	PLP-LIF	Droege and Tully (1987)	295–491
6.04×10^{-4}	1.52	−111	9.45±0.41	491			
			46.5±9.3	1194±15	SH-RA	Bott and Cohen (1989)	
			4.84±0.10	296±2	RR [relative to k(*n*-nonane) = 9.67×10^{-12}]	Kramp and Paulson (1998)	
			4.85±0.09	296±2	RR [relative to k(propene) = 2.66×10^{-11}][a]	Kramp and Paulson (1998)	
			4.86±0.21	296±2	RR [relative to k(*trans*-2-butene) = 6.48×10^{-11}][a]	Kramp and Paulson (1998)	
			4.34±0.05	296±2	RR [relative to k(1,3-butadiene) = 6.72×10^{-11}][a]	Kramp and Paulson (1998)	

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Table 52. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			5.89±0.26	300	DF-LIF	Donahue et al. (1998)	299–395
			6.35±0.59	325			
			6.18±0.19	340			
			7.64±0.23	360			
			7.25±0.38	375			
			7.53±0.45	390			
			4.34	273	RR [relative to	DeMore and Bayes (1999)	273–423
			4.68	292	$k(n\text{-butane}) =$		
			4.90	310	1.81×10^{-17}		
			5.23	326	$T^2 e^{114/T}$]		
			5.99	348			
			5.99	354			
			6.55	373			
			7.30	398			
			7.87	423			
			4.39	277	RR [relative to	DeMore and Bayes (1999)	277–360
			5.47	318	$k(n\text{-hexane}) =$		
			5.99	338	2.54×10^{-14}		
			6.41	360	$T e^{-112/T}$]		

[a] From Atkinson (1997).

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Table 53. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclopentane-d_{10}

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			1.83 ± 0.08	295	PLP-LIF	Droege and Tully (1987)	295–602
			2.46 ± 0.11	342			
			3.33 ± 0.15	401			
			4.81 ± 0.21	491			
4.50×10^{-3}	1.21	–257	6.75 ± 0.29	602			

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Table 54. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclohexane

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			7.95 ± 0.44	295	FP-KS	Greiner (1970)	295–497
			8.40 ± 0.55	338			
			7.71 ± 0.72	338			
			11.8 ± 0.6	370			
			9.93 ± 0.24	373			
			10.4 ± 0.6	425			
			10.1 ± 0.6	425			
23.5		319 ± 73	12.4 ± 0.4	497			
			6.9 ± 1.8	298	RR [relative to k(CO)=1.55 × 10^{-13}]	Gorse and Volman (1974)	
			6.6	303	RR [relative to k(*cis*-2-butene) = 5.49 × 10^{-11}][a]	Wu et al. (1976)	
			6.89 ± 0.21	299 ± 2	RR [relative to k(*n*-hexane) = 5.22 × 10^{-12}]	Atkinson et al. (1982a)	
			6.95 ± 0.05	299 ± 2	RR [relative to k(*n*-butane) = 2.37 × 10^{-12}]	Atkinson et al. (1982a)	
			7.07 ± 0.42	299 ± 2	RR [relative to k(propene) = 2.62 × 10^{-11}][a]	Atkinson et al. (1983b)	
			6.86 ± 0.10	300 ± 3	RR [relative to k(*n*-butane) = 2.38 × 10^{-12}]	Tuazon et al. (1983)	
			5.24 ± 0.36	295	PR-RA	Nielsen et al. (1986)	
			5.78 ± 0.42	297.6 ± 0.4	RR [relative to k(*n*-butane) = 2.35 × 10^{-12}]	Edney et al. (1986)	
			8.6 ± 0.8	296 ± 2	DF-RF	Bourmada et al. (1987)	

Table 54. Continued

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			7.14 ± 0.31	292	PLP-LIF	Droege and Tully (1987)	292–491
			8.49 ± 0.37	342			
			10.1 ± 0.44	401			
1.09×10^{-3}	1.47	−125	12.9 ± 0.56	491			
			7.07 ± 0.35	~298[b]	RR [relative to k(ethene) = 8.52×10^{-12}][a]	Japar et al. (1990)	
			6.69 ± 0.40	296 ± 2	RR [relative to k(*n*-butane) = 2.33×10^{-12}]	Atkinson and Aschmann (1992)	
			6.89	297 ± 2	RR [relative to k(*n*-hexane) = 5.17×10^{-12}]	Sommerlade et al. (1993)	
			6.7 ± 0.9	298	DF-LIF	Saunders et al. (1994)	
			7.6 ± 0.8	300	DF-LIF	Donahue et al. (1996)	
			7.33 ± 0.10	296 ± 2	RR [relative to k(toluene) = 5.67×10^{-12}][c]	Kramp and Paulson (1998)	
			6.76 ± 0.07	296 ± 2	RR [relative to k(1,3-butadiene) = 6.72×10^{-11}][a]	Kramp and Paulson (1998)	
			7.16 ± 0.07	296 ± 2			

Table 54. Continued

$10^{12} \times A$ (cm^3 molecule^{-1} s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 molecule^{-1} s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			6.89 ± 0.21	296 ± 2	RR [relative to k(*trans*-2-butene) = 6.48×10^{-11}][a]	Kramp and Paulson (1998)	
			7.66 ± 0.23	300	DF-LIF	Donahue et al. (1998)	299–394
			7.68 ± 0.23	325			
			7.84 ± 0.24	340			
			9.96 ± 0.34	360			
			9.06 ± 0.27	375			
			10.3 ± 0.6	390			
			6.66	301	RR [relative to k(propane) = 1.12×10^{-12}]	DeMore and Bayes (1999)	
			6.59	301			
			6.75	298	RR [relative to k(*n*-butane) = $1.81 \times 10^{-17} T^2 e^{114/T}$]	DeMore and Bayes (1999)	298–363
			7.77	326			
			8.49	350			
			8.91	363			
			6.83	298	RR [relative to k(*n*-pentane) = $2.52 \times 10^{-17} T^2 e^{158/T}$]	DeMore and Bayes (1999)	298–368
			7.39	312			
			8.20	338			
			9.25	368			

[a] From Atkinson (1997).
[b] Room temperature; assumed to be ~298 K.
[c] From Calvert et al. (2002).

Table 55. Rate constants and temperature-dependent parameters for the reaction of OH radicals with cyclohexane-d_{12}

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	n	B(K)	$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (K)
			2.76 ± 0.12	292	PLP-LIF	Droege and Tully (1987)	292–603
			3.64 ± 0.16	342			
			4.83 ± 0.21	401			
			6.94 ± 0.30	491			
3.48×10^{-4}	1.62	−56	9.78 ± 0.42	603			

Table 56. Rate constants for the reaction of OH radicals with methylcyclohexane

$10^{12} \times A$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
9.64 ± 0.24	297 ± 2	RR [relative to k(*n*-butane) = 2.34×10^{-12}]	Atkinson et al. (1984)

Table 57. Rate constants for the reaction of OH radicals with *n*-butylcyclohexane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
14.7 ± 0.5	296 ± 2	RR[relative to k(*n*-octane) = 8.07×10^{-12}]	Aschmann et al. (2001)

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Table 58. Rate constants for the reaction of OH radicals with cycloheptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (k)
13.1 ± 2.1	298 ± 2	FP-RA	Jolly et al. (1985)	
12.0 ± 0.3	300	DF-LIF	Donahue et al. (1998)	298–388
13.4 ± 0.4	325			
13.3 ± 0.4	340			
14.9 ± 0.4	375			
16.4 ± 1.4	390			

Table 59. Rate constants for the reaction of OH radicals with cyclooctane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference	Temperature Range (k)
13.4 ± 0.4	300	DF-LIF	Donahue et al. (1998)	298–387
15.0 ± 0.4	325			
14.9 ± 0.4	340			
16.6 ± 0.5	375			
19.1 ± 0.6	390			

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Table 60. Rate constants for the reaction of OH radicals with bicyclo[2.2.1]heptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
5.12 ± 0.13	299 ± 2	RR [relative to k(cyclohexane) = 7.00 × 10^{-12}]	Atkinson et al. (1983c)

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Table 61. Rate constants for the reaction of OH radicals with bicyclo[2.2.2]octane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
13.7 ± 1.0	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

Table 62. Rate constants for the reaction of OH radicals with bicyclo[3.3.0]octane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
10.3 ± 0.5	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

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Table 63. Rate constants for the reaction of OH radicals with *cis*-bicyclo[4.3.0]nonane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
16.0 ± 1.2	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

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Table 64. Rate constants for the reaction of OH radicals with *trans*-bicyclo[4.3.0]nonane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
16.5 ± 1.2	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

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Table 65. Rate constants for the reaction of OH radicals with *cis*-bicyclo[4.4.0]decane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
18.6 ± 1.3	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

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Table 66. Rate constants for the reaction of OH radicals with *trans*-bicyclo[4.4.0]decane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
19.0 ± 1.2	299 ± 2	RR [relative to k(cyclohexane) = 7.00×10^{-12}]	Atkinson et al. (1983c)

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Table 67. Rate constants for the reaction of OH radicals with tricyclo[5.2.1.$0^{2,6}$]decane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
10.6 ± 0.4	299 ± 2	RR [relative to k(cyclohexane) = 7.00 × 10^{-12}]	Atkinson et al. (1983c)

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Table 68. Rate constants for the reaction of OH radicals with tricyclo[3.3.1.1^{3,7}]decane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
21.5 ± 1.9	299 ± 2	RR [relative to k(cyclohexane) = 7.00 × 10^{-12}]	Atkinson et al. (1983c)

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Table 69. Rate constants for the reaction of OH radicals with *trans*-pinane; (1R, 2R)-2,6,6-trimethylbicyclo[3.3.1]heptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
12.4 ± 1.0	296 ± 2	RR [relative to $k(n\text{butane}) = 2.33 \times 10^{-12}$]	Atkinson and Aschmann (1992)

Table 70. Rate constants for the reaction of OH radicals with tricyclene; 1,7,7-trimethyltricyclo[2.2.1.$0^{2,6}$]heptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
2.66 ± 0.21	296 ± 2	RR [relative to $k(n\text{butane}) = 2.33 \times 10^{-12}$]	Atkinson and Aschmann (1992)

Table 71. Rate constants for the reaction of OH radicals with quadricyclane; quadricyclo[2.2.1.$0^{2,6}$.$0^{3,5}$]heptane

$10^{12} \times k$ (cm^3 $molecule^{-1}$ s^{-1})	at T(K)	Technique	Reference
1.70 ± 0.16	296 ± 2	RR [relative to $k(n\text{butane}) = 2.33 \times 10^{-12}$]	Atkinson and Aschmann (1992)

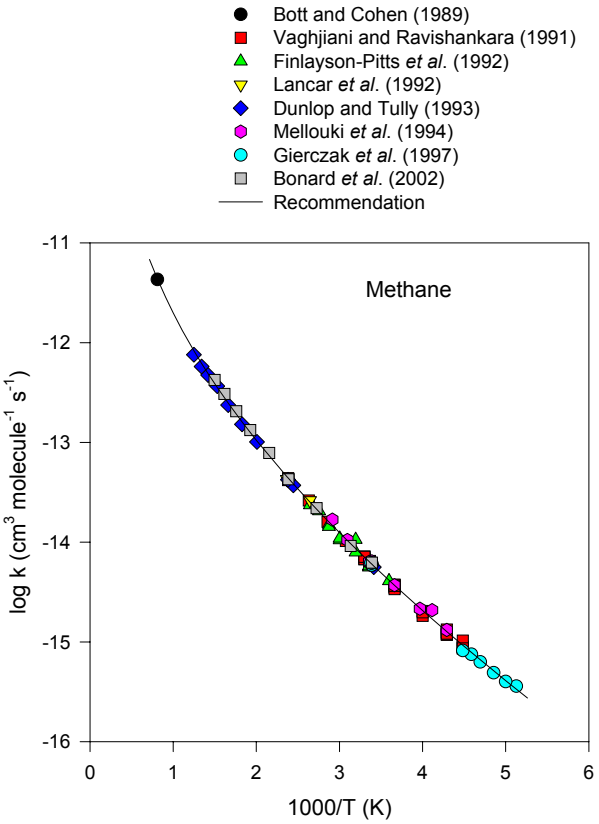

Fig. 1. Arrhenius plot of selected rate data for the reaction of OH radicals with methane.

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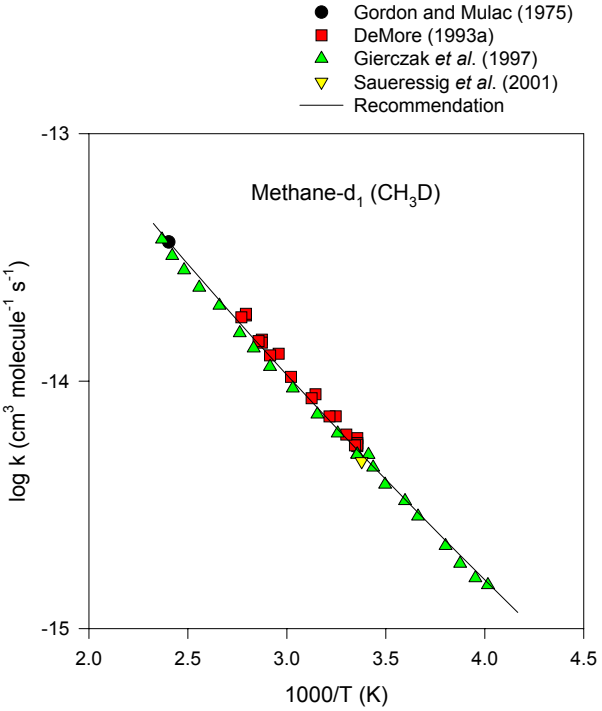

Fig. 2. Arrhenius plot of the rate data for the reaction of OH radicals with methane-d_1 (CH_3D).

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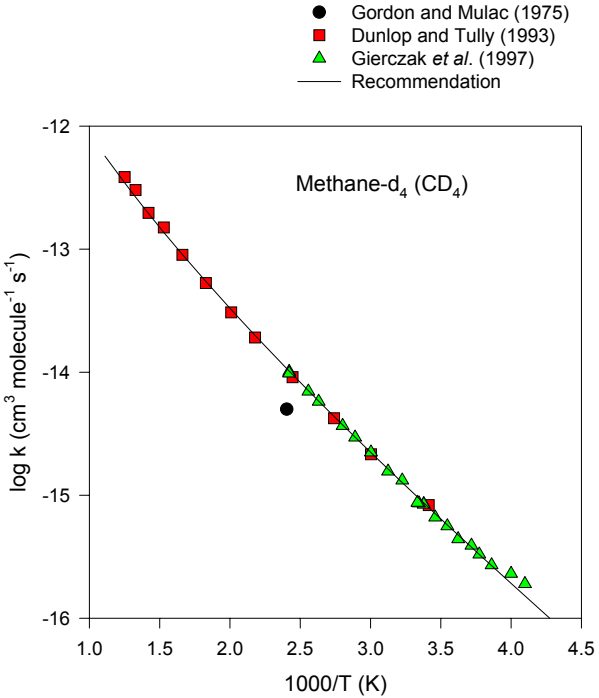

Fig. 3. Arrhenius plot of the rate data for the reaction of OH radicals with methane-d_4 (CD_4).

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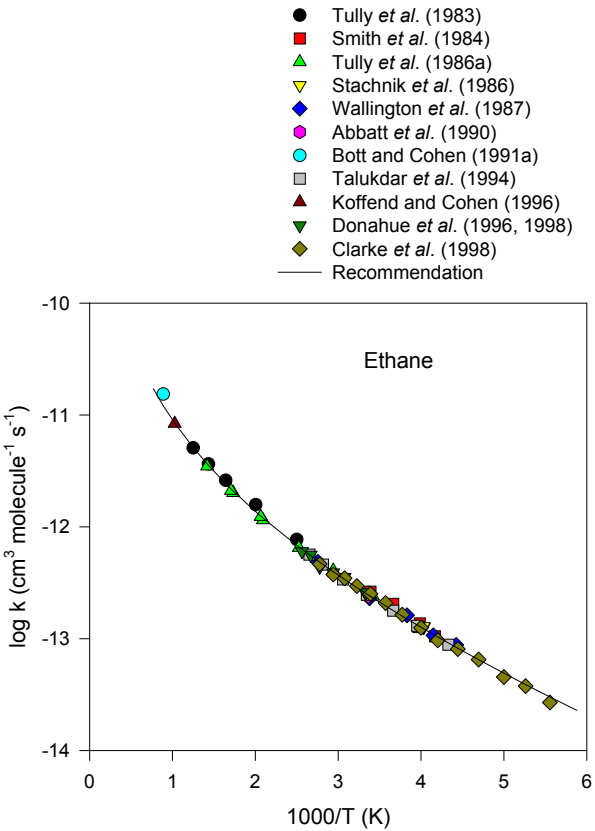

Fig. 4. Arrhenius plot of selected rate data for the reaction of OH radicals with ethane.

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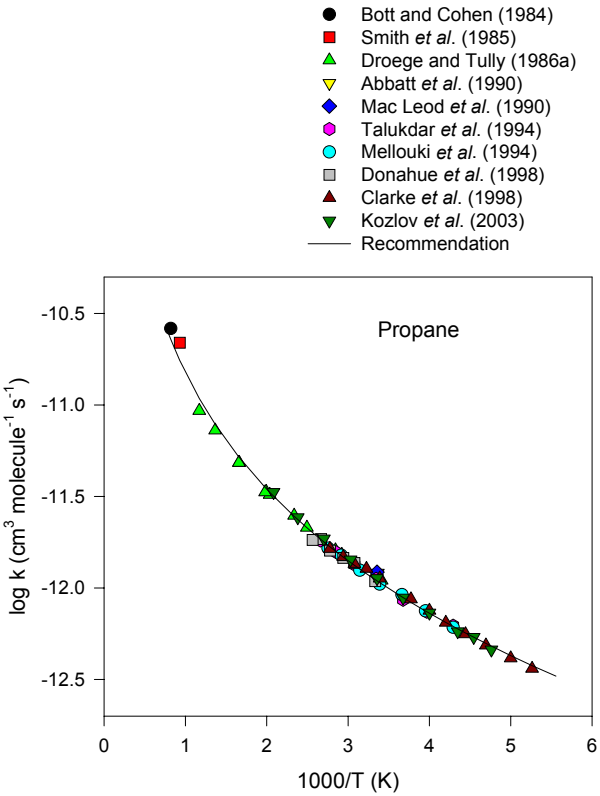

Fig. 5. Arrhenius plot of selected rate data for the reaction of OH radicals with propane.

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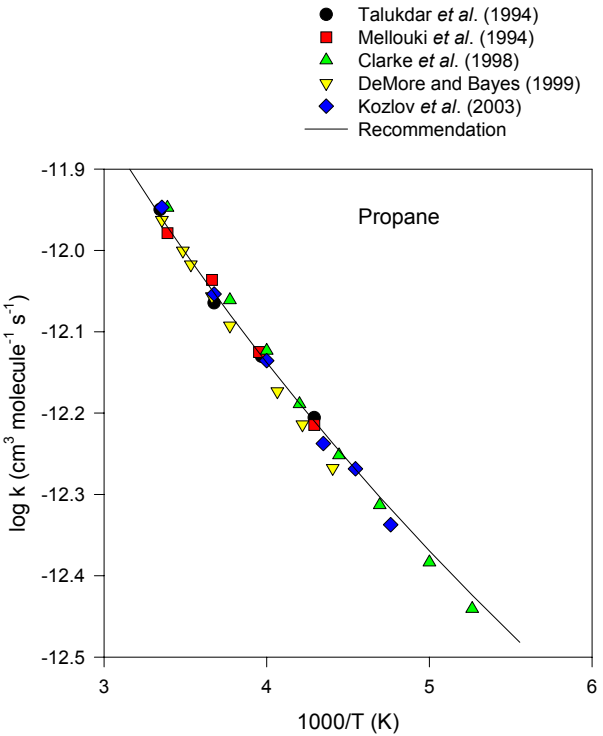

Fig. 6. Arrhenius plot of selected rate data for the reaction of OH radicals with propane at temperatures < 300 K.

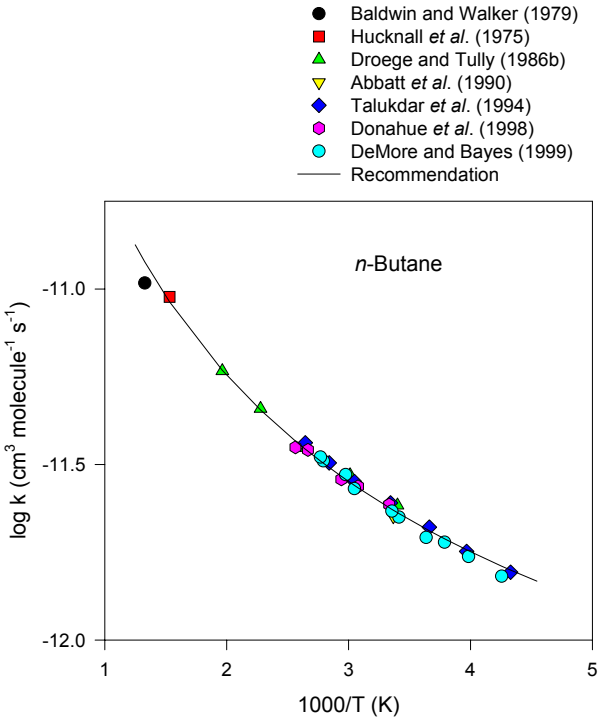

Fig. 7. Arrhenius plot of selected rate data for the reaction of OH radicals with *n*-butane.

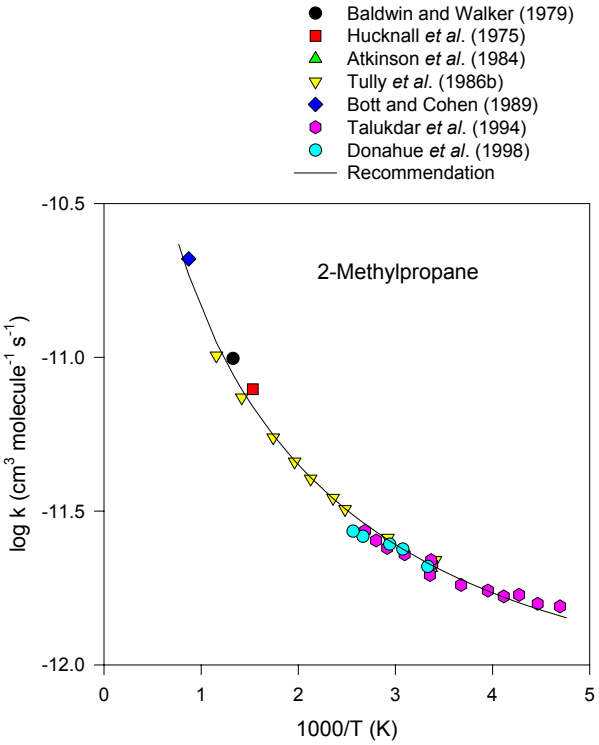

Fig. 8. Arrhenius plot of selected rate data for the reaction of OH radicals with 2-methylpropane.

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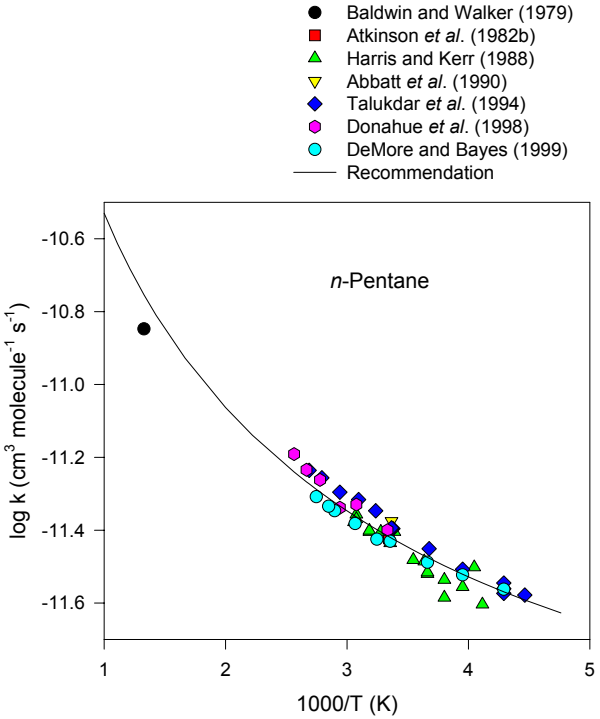

Fig. 9. Arrhenius plot of selected rate data for the reaction of OH radicals with *n*-pentane.

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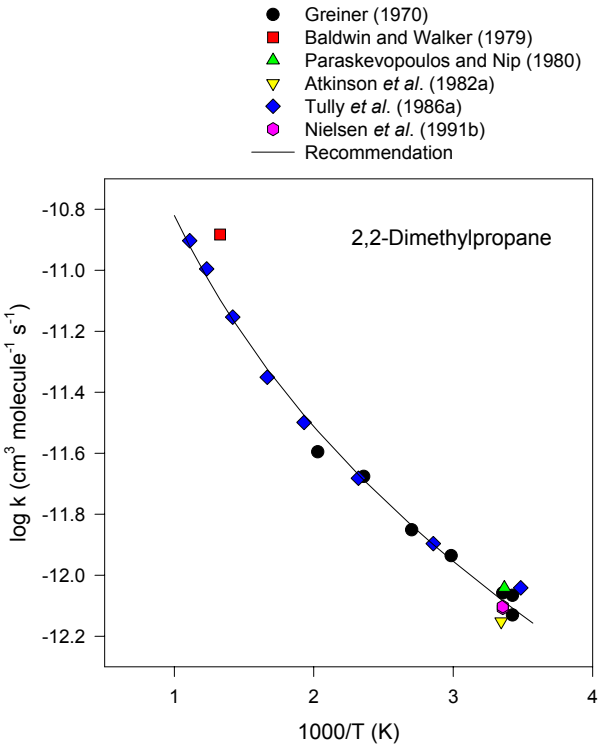

Fig. 10. Arrhenius plot of selected rate data for the reaction of OH radicals with 2,2-dimethylpropane.

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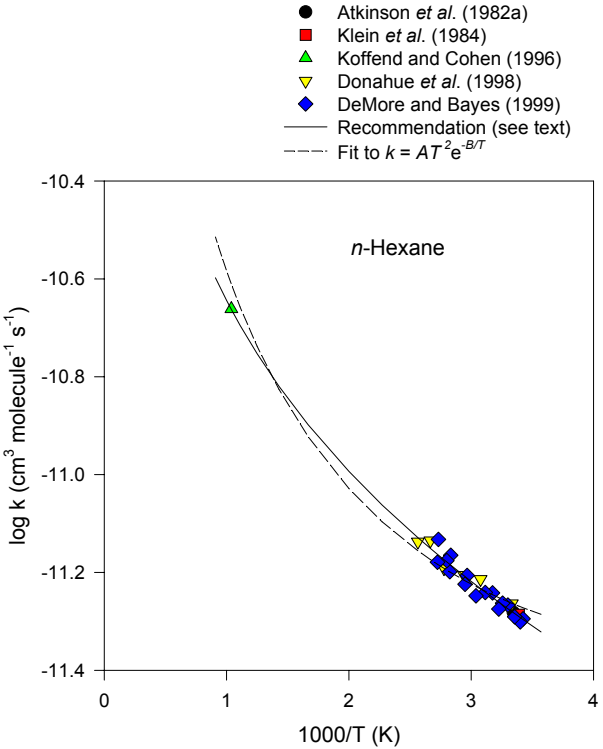

Fig. 11. Arrhenius plot of selected rate data for the reaction of OH radicals with *n*-hexane.

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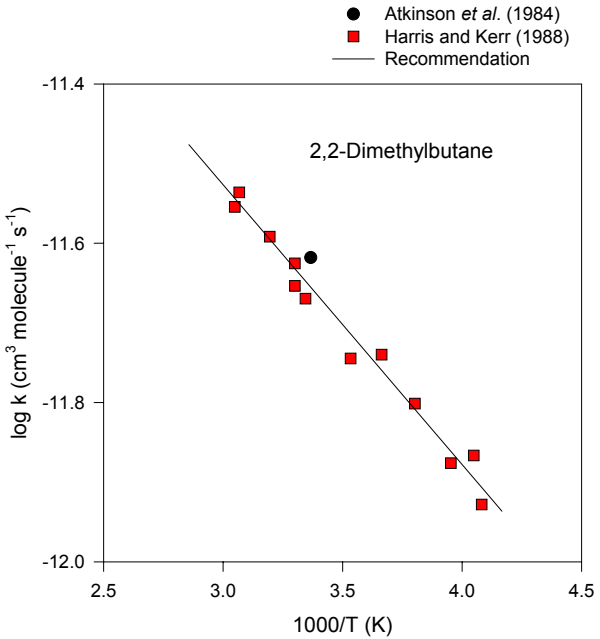

Fig. 12. Arrhenius plot of the rate data for the reaction of OH radicals with 2,2-dimethylbutane.

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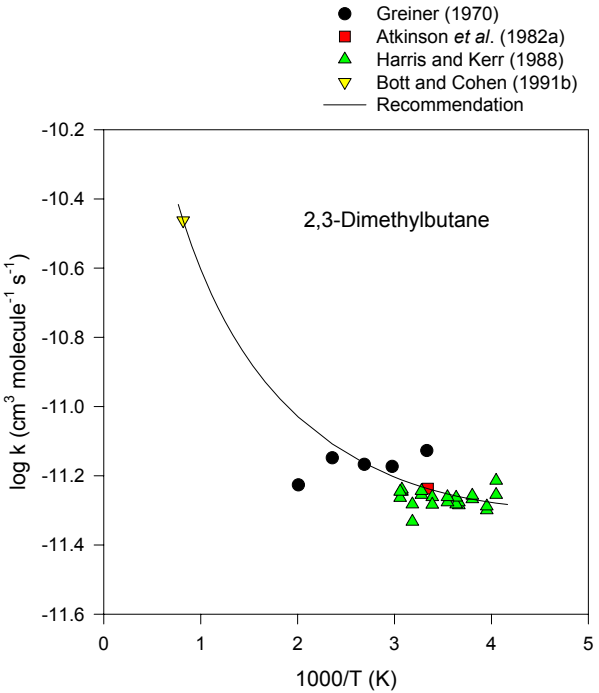

Fig. 13. Arrhenius plot of selected rate data for the reaction of OH radicals with 2,3-dimethylbutane.

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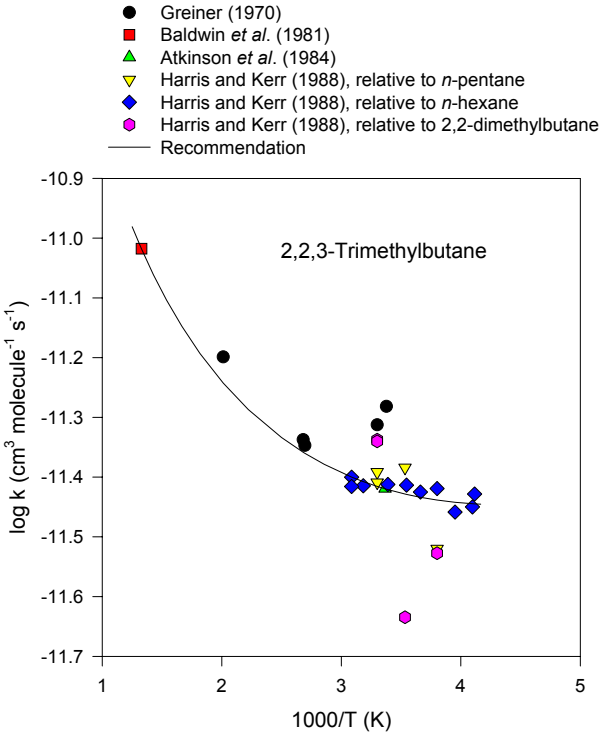

Fig. 14. Arrhenius plot of selected rate data for the reaction of OH radicals with 2,2,3-trimethylbutane.

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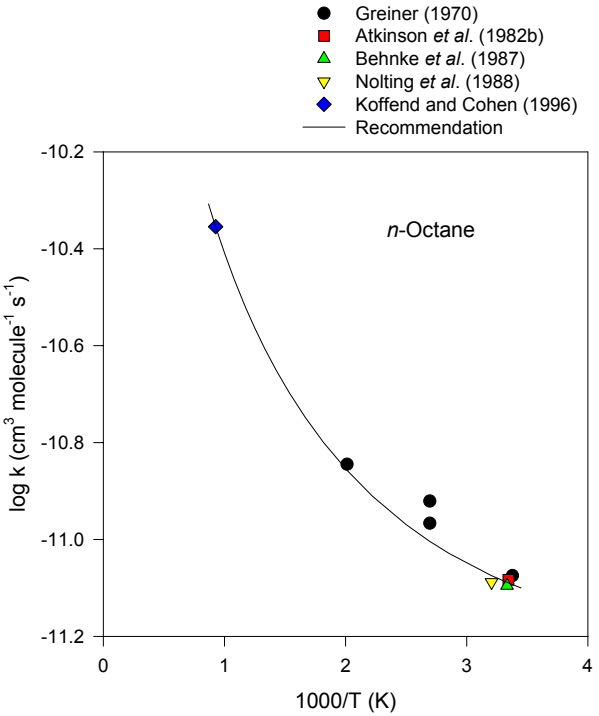

Fig. 15. Arrhenius plot of the rate data for the reaction of OH radicals with *n*-octane.

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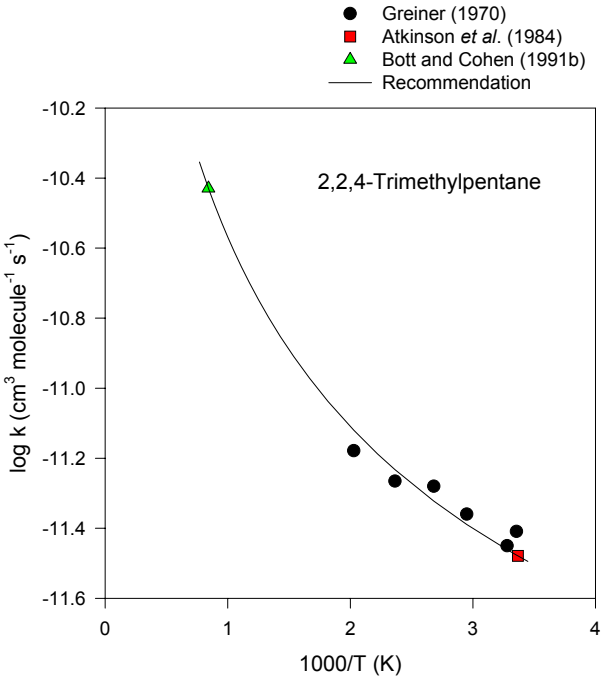

Fig. 16. Arrhenius plot of the rate data for the reaction of OH radicals with 2,2,4-trimethylpentane.

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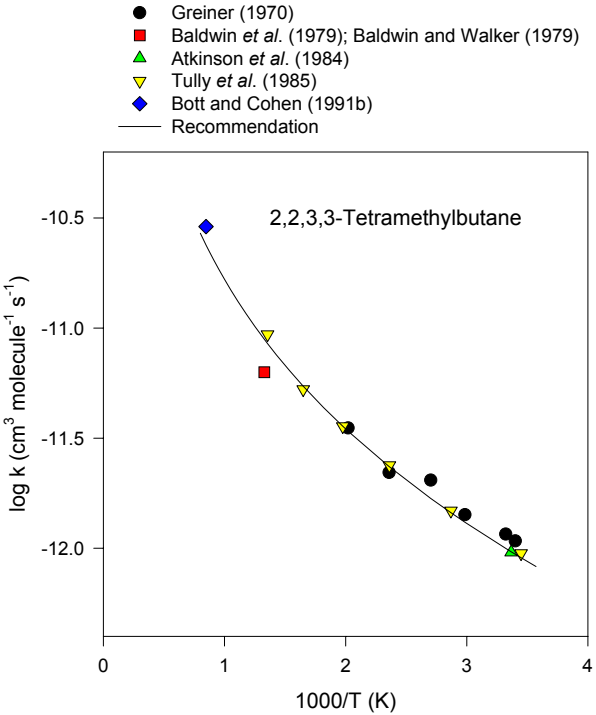

Fig. 17. Arrhenius plot of the rate data for the reaction of OH radicals with 2,2,3,3-tetramethylbutane.

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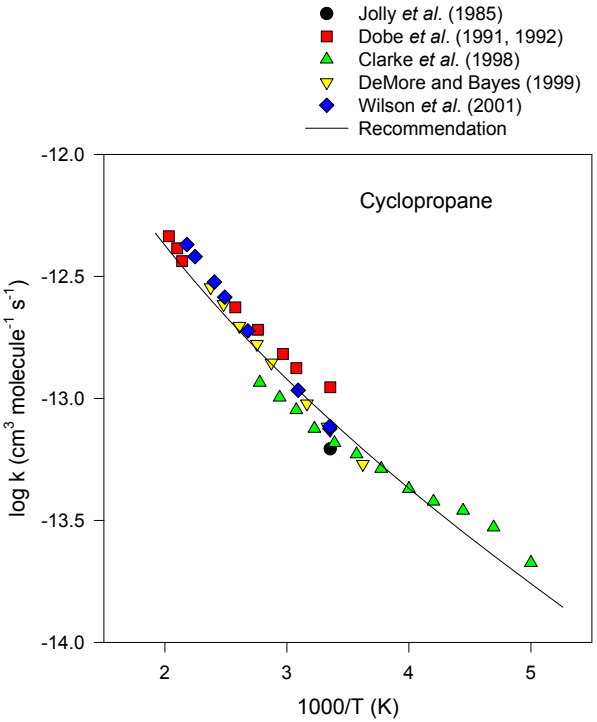

Fig. 18. Arrhenius plot of selected rate data for the reaction of OH radicals with cyclopropane.

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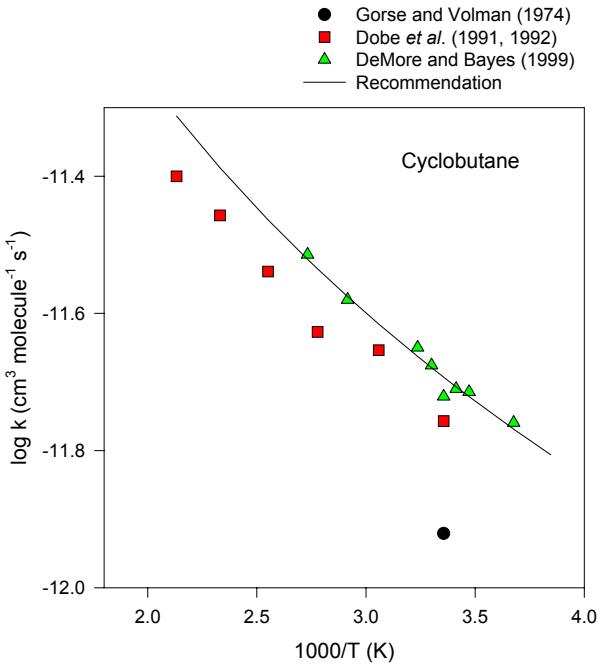

Fig. 19. Arrhenius plot of the rate data for the reaction of OH radicals with cyclobutane.

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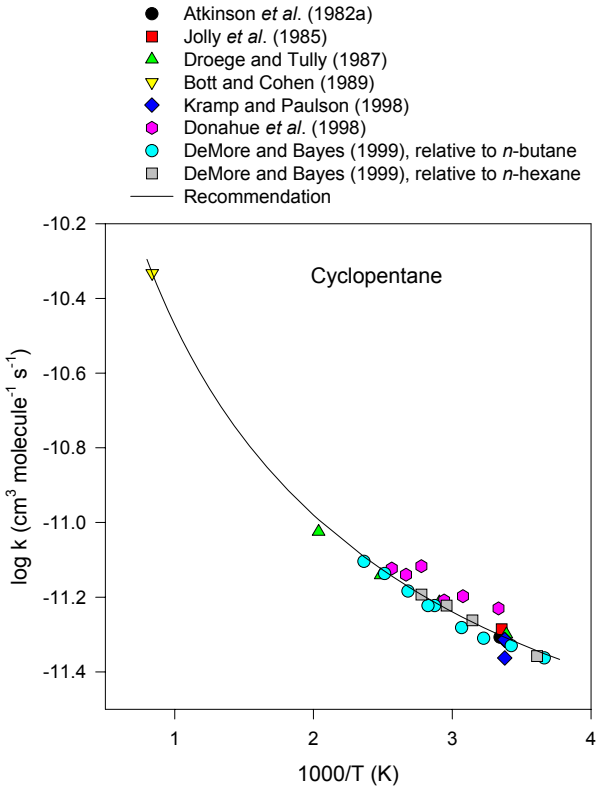

Fig. 20. Arrhenius plot of selected rate data for the reaction of OH radicals with cyclopentane.

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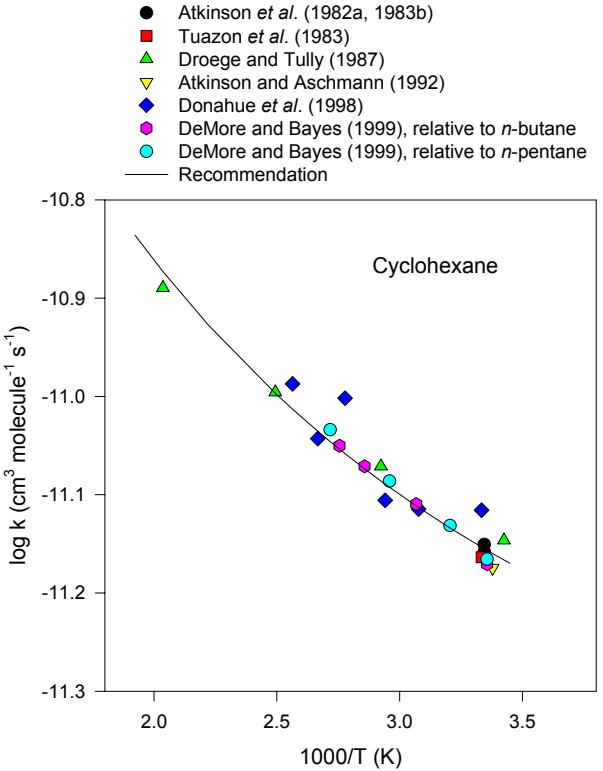

Fig. 21. Arrhenius plot of selected rate data for the reaction of OH radicals with cyclohexane.

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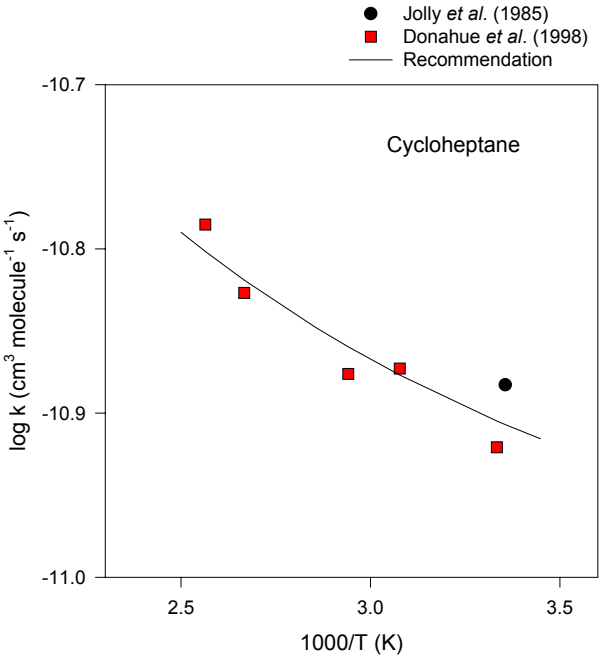

Fig. 22. Arrhenius plot of the rate data for the reaction of OH radicals with cycloheptane.

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